On Z_n graded Baker–Campbell–Hausdorff formulas and coset space parametrizations

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We present a generalization of the BCH formula, $\exp \Delta \exp \Gamma = \exp(\Delta + \Gamma + \frac{1}{2}[\Delta,\Gamma] + \cdots)$, involving n factors on the right, linear in Δ and to all orders in Γ. The result is applicable to coset geometries involving Z_n graded algebras and superalgebras. In the Z_2 case expressions are obtained for group transformations in the spaces $S^{n-1} = \mathrm{O}(n)/\mathrm{O}(n-1)$, $\mathrm{CP}^n = \mathrm{SU}(n+1)/\mathrm{U}(n)$, $\mathrm{OSp}(1/n)/\mathrm{Sp}(n)$, and $\mathrm{SU}(n/1)/\mathrm{U}(n)$.

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I. INTRODUCTION

Due to renewed interest in the interpretation of Kaluza–Klein theories[1] and their dimensional reduction, coset spaces have again become a research subject.[2] When dealing with such spaces, a convention-dependent particular parametrization of cosets is frequently required. Recently Delbourgo and Jarvis,[3] using a Wigner-type convention[4] for coset actions, derived a generalization of the famous Baker–Campbell–Hausdorff (BCH) formula

$$\exp A \exp B = \exp(A + B + \tfrac{1}{2}[A,B] \cdots).$$

Their generalization has two factors on the right, one containing all brackets of odd order and the other having the even ones. The new formula is applicable to all Z_2 graded algebras (including superalgebras) and is valid for infinitesimal A and finite B. In this paper we extend their result to the case of n factors on the right, appropriate to Z_n graded algebras and superalgebras (Sec. II). The Z_2 result is applied to several coset spaces in Sec. III.

II. DERIVATION OF THE Z_n FORMULA

Let $G = G_1 \oplus G_2 \oplus \cdots \oplus G_n$ be a real Z_n graded algebra. If we denote by J_j generators in the subspace G_j then we have the generic commutators

$$\begin{aligned}
&[J_n, J_n] = iJ_n,\\
&[J_n, J_j] = iJ_j, \quad j = 1,2,3,\ldots,n-1, \qquad (1)\\
&[J_j, J_k] = iJ_{(j+k)\bmod n}.
\end{aligned}$$

An arbitrary group transformation may be expressed as the product of a coset space action and a little group action,

$$[\exp(i\gamma_1 J_1)\exp(i\gamma_2 J_2)\cdots\exp(i\gamma_{n-1}J_{n-1})]\exp(i\gamma_n J_n). \quad (2)$$

We seek to write the product of two coset actions in the above form. As an initial step in this direction we take the product of two coset actions to be

$$\exp\Delta \exp\Gamma = \exp(i\delta_1 J_1)\exp(i\gamma_1 J_1), \quad (3)$$

where δ_1 is infinitesimal. The problem now is to determine the coefficients a_i such that

$$\exp\Delta \exp\Gamma = \exp(\Gamma + \partial J_1)\exp(\partial J_2) \times \exp(\partial J_3)\cdots\exp(\partial J_n), \quad (4)$$

with

$$\partial J_i = \sum_{j=0}^{\infty} a_{jn+i-1}[\Delta,\Gamma]_{jn+i-1}, \quad (5)$$

and where $[\Delta,\Gamma]_n$ stands for the n-fold commutator $[[[\cdots[\Delta,\Gamma]\ldots,\Gamma], [\Delta,\Gamma]_0 = \Delta$. To first order in Δ,

$$\begin{aligned}
&\exp(-\Gamma)(1+\Delta)\exp(\Gamma)\\
&\quad = \exp(-\Gamma)\exp(\Gamma + \partial J_1)(1 + \partial J_2 + \cdots + \partial J_n). \qquad (6)
\end{aligned}$$

Both left- and right-hand sides can be easily calculated using the commutation relations

$$\exp(-A)\exp(A + \partial A) = 1 + \sum_{n=0}^{\infty}[\partial A, A]_n/(n+1)!,$$

$$\exp(-A)B\exp(A) = \sum_{n=0}^{\infty}[B,A]_n/n!$$

The result is

$$\begin{aligned}
1 + \sum_{p=0}^{\infty}[\Delta,\Gamma]_p/p! &= 1 + \sum_{p=0}^{\infty}\sum_{\alpha=0}^{\infty} a_{\alpha n}[\Delta,\Gamma]_{\alpha n+p}/(p+1)!\\
&\quad + \sum_{\alpha=0}^{\infty} a_{\alpha n+1}[\Delta,\Gamma]_{\alpha n+1} + \cdots\\
&\quad + \sum_{\alpha=0}^{\infty} a_{\alpha n+n-1}[\Delta,\Gamma]_{\alpha n+n-1}. \qquad (7)
\end{aligned}$$

Comparing coefficients of the multiple commutators we obtain the recursion relations

$$1/(kn)! = a_{kn} + \sum_{j=1}^{\infty} a_{(k-j)n}/(jn+1)!, \quad (8a)$$

$$1/(kn+c)! = a_{kn+c} + \sum_{j=0}^{\infty} a_{(k-j)n}/(jn+c+1)!, \quad (8b)$$

$$1 \leqslant c \leqslant n-1,$$

where we have defined $a_{-i} = 0$, $i \in Z^+$. Let the generating functions for successive coefficients be provided by

$$a(x) = \sum_{k=0}^{\infty} a_{kn}x^{kn}, \quad (9a)$$

$$b_c(x) = \sum_{k=0}^{\infty} a_{kn+c}x^{kn+c}. \quad (9b)$$

Substituting for the a_i from Eqs. (8a) and (8b) gives

$$a(x) = x\sum_{k=0}^{\infty}(x^{kn}/(kn)!)\Big/\sum_{k=0}^{\infty}(x^{kn+1}/(kn+1)!), \quad (10a)$$

$$b_c(x)=\sum_{k=0}^{\infty}(x^{kn+c}/(kn+c)!)$$
$$-a(x)\sum_{k=0}^{\infty}(x^{kn+c}/(kn+c+1)!),\quad 1\leqslant c\leqslant n-1. \tag{10b}$$

Taking the limit $n\to\infty$ results in the generating functions

$$a(x)=1,\quad b_c(x)=cx^c/(c+1)!.$$

Hence

$$\exp\Delta\,\exp\Gamma=\exp(\Gamma+\Delta)\exp(\tfrac{1}{2}[\Delta,\Gamma])\exp([\Delta,\Gamma]_2/3)\cdots$$
$$\exp(c[\Delta,\Gamma]_c/(c+1)!)\cdots, \tag{11}$$

which is just the Zassenhaus formula[5] for infinitesimal Δ. Setting $n=1$ we have

$$a(x)=xe^x/(e^x-1), \tag{12}$$

in agreement with the Bagger and Wess[6] infinitesimal form of the BCH formula. In the case $n=2$,

$$\exp\Delta\,\exp\Gamma=\exp(\Gamma+\sum_{k=0}^{\infty}a_{2k}[\Delta,\Gamma]_{2k})$$
$$\times\exp(\sum_{k=0}^{\infty}b_{2k+1}[\Delta,\Gamma]_{2k+1}). \tag{13}$$

The generating functions for the coefficients are given by

$$a(x)=x\coth(x), \tag{14a}$$
$$b(x)=\tanh(x/2), \tag{14b}$$

reproducing the results of Delbourgo and Jarvis.[3] It is this Z_2 case to which we now turn our attention in the following examples.

III. EXAMPLES OF THE Z_2 GRADING FORMULA

A. $S^{n-1}=\mathrm{O}(n)/\mathrm{O}(n-1)$

For this case we denote the generators of O(n) by $T_{\alpha\beta}$ for $\alpha,\beta=1,2,\ldots,n$. The T's are antisymmetric and obey the commutation relation

$$[T_{\alpha\beta},T_{\gamma\delta}]=i(\delta_{\alpha\gamma}T_{\beta\delta}+\delta_{\beta\delta}T_{\alpha\gamma}-\delta_{\alpha\delta}T_{\beta\gamma}-\delta_{\beta\gamma}T_{\alpha\delta}). \tag{15}$$

The generators of O($n-1$) are relabeled as J_{kj}, $k,j=1,2,\ldots,n-1$ and the remaining ones are labeled as $K_j=T_{jn}$.

With $\Gamma=i\mathbf{K}\cdot\boldsymbol{\gamma}$ and $\Delta=i\mathbf{K}\cdot\boldsymbol{\delta}$ where the δ_j are infinitesimal, it is a trivial task to evaluate the multiple commutators to be

$$[\Delta,\Gamma]_{2p+1}=-i(-\gamma^2)^p\delta_kJ_{kj}\gamma_j, \tag{16a}$$
$$[\Delta,\Gamma]_{2p}=(-\gamma^2)^{p-1}((\boldsymbol{\delta}\cdot\boldsymbol{\gamma})\Gamma-\gamma^2\Delta),\quad p\geqslant 1. \tag{16b}$$

Inserting these expressions in the Z_2 grading formula (13) and using (14) gives

$$\exp\Delta\,\exp\Gamma$$
$$=\exp\{\Gamma+\boldsymbol{\delta}\cdot\boldsymbol{\gamma}\Gamma(1-\gamma\cot(\gamma))/\gamma^2+\cot(\gamma)\gamma\Delta\}$$
$$\times\exp(-i\delta_kJ_{kj}\gamma_j\tan(\gamma/2)/\gamma), \tag{17}$$

which is a trivial generalization of the O(4)/O(3) result given by Delbourgo and Jarvis.[3]

B. $\mathrm{CP}^n=\mathrm{SU}(n+1)/\mathrm{U}(n)$

In this example we adopt the standard Gell-Mann notation and denote the Hermitian generators of SU($n+1$) by F_i, $i=1,2,\ldots,(n+1)^2-1$. The maximal subalgebra U(n) is assumed to be generated by $F_1,F_2,\ldots,F_{n^2-1}$ and $F_{(n+1)^2-1}$. As we are dealing with a complex projective space, we combine the coset generators of CP^n into an n-dimensional spinor, denoted by K. Similarly we form a spinor γ from the real coset parameters γ_j, $j=n^2,\ldots,(n+1)^2-2$. This gives

$$\Gamma=i(F_{n^2}\gamma_{n^2}+\cdots+F_{(n+1)^2-2}\gamma_{(n+1)^2-2}),$$
$$=i(\bar{\gamma}K+\bar{K}\gamma)/2, \tag{18}$$

where

$$\gamma=\begin{pmatrix}\gamma_{n^2}-i\gamma_{n^2+1}\\ \cdot\\ \cdot\\ \cdot\\ \gamma_{(n+1)^2-3}-i\gamma_{(n+1)^2-2}\end{pmatrix},$$
$$K=\begin{pmatrix}F_{n^2}-iF_{n^2+1}\\ \cdot\\ \cdot\\ \cdot\\ F_{(n+1)^2-3}-iF_{(n+1)^2-2}\end{pmatrix}. \tag{19}$$

With the further definition

$$J_{\mathrm{SU}(n+1)}=\sum_{i=1}^{n^2-1}F_i\lambda_i+(2(n+1)/n)^{1/2}F_{n(n+2)}I_n, \tag{20}$$

where λ_i is the ith Gell-Mann matrix of SU(n) and $I(n)$ is the $n\times n$ unit matrix, the SU($n+1$) algebra can be expressed in the form

$$[\Delta,\Gamma]_1=\tfrac{1}{4}(\bar{\delta}J\gamma-\bar{\gamma}J\delta), \tag{21a}$$
$$[\Delta,\Gamma]_2=-\tfrac{1}{4}y^2\Delta+(\bar{\gamma}\delta+\bar{\delta}\gamma)\Gamma/8$$
$$+3i(\bar{\delta}\gamma-\bar{\gamma}\delta)(\bar{K}\gamma-\bar{\gamma}K)/16, \tag{21b}$$
$$[\bar{K}\gamma-\bar{\gamma}K,\Gamma]=i\bar{\gamma}J\gamma, \tag{21c}$$
$$[\bar{\gamma}J\gamma,\Gamma]=iy^2(\bar{K}\gamma-\bar{\gamma}K), \tag{21d}$$

where $y^2=\bar{\gamma}\gamma$. (21e)

The multiple commutators are given by

$$[\Delta,\Gamma]_{2p+1}=u_py^{2p}(\bar{\delta}J\gamma-\bar{\gamma}J\delta)+v_py^{2p-2}(\bar{\delta}\gamma-\bar{\gamma}\delta)\bar{\gamma}J\gamma, \tag{22a}$$

$$[\Delta,\Gamma]_{2p}=x_py^{2p}\Delta+y^{2p-2}(w_p(\bar{\gamma}\delta+\bar{\delta}\gamma)\Gamma$$
$$+iz_p(\bar{\delta}\gamma-\bar{\gamma}\delta)(\bar{K}\gamma-\bar{\gamma}K)),\quad p\geqslant 1. \tag{22b}$$

The various coefficients may be evaluated using recurrence relations, with the outcome

$$x_p=(-\tfrac{1}{4})^p,\quad u_p=-(-\tfrac{1}{4})^{p+1},\quad w_p=-\tfrac{1}{2}(-\tfrac{1}{4})^p,$$
$$z_p=-v_p=(-\tfrac{1}{4})^{p+1}(4^p-1). \tag{23}$$

Using these expressions in (13) gives the concise formula

$$\exp\Delta\,\exp\Gamma$$
$$=\exp\{\Gamma+\tfrac{1}{2}y\Delta\cot(y/2)+\tfrac{1}{4}[(\bar{\gamma}\delta+\bar{\delta}\gamma)\Gamma(2-y\cot(y/2))$$
$$+i(\bar{\gamma}\delta-\bar{\delta}\gamma)(\bar{K}\gamma-\bar{\gamma}K)(y\cot(y)-\tfrac{1}{2}y\cot(y/2))]/y^2\}$$
$$\times\exp\{\tfrac{1}{4}(\bar{\gamma}\delta-\bar{\delta}\gamma)\bar{\gamma}J\gamma(2\tan(y/4)-\tan(y/2))$$
$$+\tfrac{1}{2}(\bar{\delta}J\gamma-\bar{\gamma}J\delta)\tan(y/4)/y\}. \tag{24}$$

Computationally speaking, the calculations proved to be simpler if the matrix form of the SU($n+1$) generators was used in preference to the Gell-Mann form. The alternative generators ($T_{\alpha\beta}$) obey the commutation relation

$$[T_{\alpha\beta},T_{\gamma\delta}] = \delta_{\gamma\beta}T_{\alpha\delta} - \delta_{\alpha\delta}T_{\gamma\beta}, \tag{25}$$

where $\alpha, \beta, \gamma, \delta = 1, 2,\dots,n+1$, and they satisfy $(T_{\alpha\beta})^\dagger = T_{\beta\alpha}$ and $\Sigma_{i=1}^{n} T_{ii} = -T_{n+1,n+1}$. Those T's that generate U(n) are denoted by J, $J_{ij} = T_{ij}$, $i,j = 1, 2,\dots,n$, while the coset generators are denoted by L: $L_i = T_{i,n+1}$, $L_{i+n} = T_{n+1,i}$. Because of the hermiticity property, the coset parameters are now complex and satisfy $\eta_i^* = \eta_{i+n}$ so that

$$\begin{aligned}\Gamma &= i(L_1\eta_1 + L_2\eta_2 + \cdots + L_n\eta_n \\ &\quad + L_1^\dagger\eta_1^* + L_2^\dagger\eta_2^* + \cdots + L_n^\dagger\eta_n^*) \\ &= i\mathbf{L}\cdot\boldsymbol{\eta}.\end{aligned} \tag{26}$$

The details of the calculation using this notation and the conversion to the previous notation are presented in the Appendix. The result is given by

$$\begin{aligned}\exp\Delta\,\exp\Gamma = \exp\big[&\Gamma + \Delta + \tfrac{1}{4}i((\eta_h\wedge\theta_h)(\delta_{kl}x^2 + \eta_l\eta_k^*)(2x\cot(2x) - 1) \\ &+ 4((\eta_k\wedge\theta_l)x^2 - (\eta_h\wedge\theta_h)\eta_k^*\eta_l)(x\cot(x) - 1))x^{-4}(\eta_k L_l - \eta_l^* L_k)\big] \\ &\times\exp\big[\tfrac{1}{2}x^{-3}((\eta_h\wedge\theta_h)\eta_i\eta_j^*(2\tan(x/2) - \tan(x)) \\ &- 2x^2(\eta_j\wedge\theta_i)\tan(x/2))(J_{ij} - \delta_{ij}T_{n+1,n+1})\big],\end{aligned} \tag{27}$$

where, to avoid confusion, we use $\Gamma = i\mathbf{L}\cdot\boldsymbol{\eta}$, $\Delta = i\mathbf{L}\cdot\boldsymbol{\theta}$ in the calculation using the alternate notation. The quantity $(\theta_j\wedge\eta_i)$ is given by

$$(\theta_j\wedge\eta_i) \equiv (\theta_j^*\eta_i - \eta_j^*\theta_i) = -(\eta_j\wedge\theta_i), \tag{28}$$

while

$$x^2 \equiv \eta_i^*\eta_i = \tfrac{1}{2}|\boldsymbol{\eta}|^2. \tag{29}$$

The indices h to l run from 1 to n with summation over repeated indices.

C. OSp(1/n)/Sp(n)

The generators of OSp(1/n) satisfy the commutation relation[7]

$$\begin{aligned}[T_{AB},T_{CD}] = {}& g_{BC}T_{AD} - [AB]g_{AC}T_{BD} \\ & - [CD]g_{BD}T_{AC} + [AB][CD]g_{AD}T_{BC},\end{aligned} \tag{30}$$

where

$$T_{AB} = -[AB]T_{BA} \tag{31a}$$

and the sign factor $[AB]$ is defined by

$$[AB] = (-1)^{(A)(B)}, \tag{31b}$$

$$(A) = \begin{cases}0 & \text{for } A = 1,\\ 1 & \text{for } 2\leqslant A\leqslant n+1.\end{cases} \tag{31c}$$

With the identification

$$\begin{aligned}K_a &= T_{1a} = -T_{a1}, \\ J_{ab} &= T_{ab} = J_{ba},\end{aligned}\qquad a,b = 2,3,\dots,n+1, \tag{32}$$

we obtain the result

$$\begin{aligned}\exp\Delta\,\exp\Gamma = \exp[&(1 + (\bar\delta\gamma)/(\bar\gamma\gamma))\Gamma + (\bar\gamma\gamma)^{1/2} \\ &\times\cot(\bar\gamma\gamma)^{1/2}\Delta - (\bar\delta\gamma)(\bar\gamma\gamma)^{-1/2}\cot(\bar\gamma\gamma)^{1/2}\Gamma] \\ &\times\exp[-\tan(\tfrac{1}{2}(\bar\gamma\gamma)^{1/2})\delta^a\gamma^b J_{ab}/(\bar\gamma\gamma)^{1/2}],\end{aligned} \tag{33}$$

where

$$\Delta = iK_a\delta^a,\quad \Gamma = iK_a\gamma^a,\quad \bar\gamma\gamma = \gamma^a g_{ab}\gamma^b. \tag{34}$$

Note that since γ is an a-number, $\bar\gamma\gamma$ is a nilpotent c-number and the power series [e.g., $\cot(\bar\gamma\gamma)^{1/2}$] terminate after a finite number of terms. The final series expansions of course involve only integral powers of $\bar\gamma\gamma$.

D. SU(n/1)/SU(n)$\times$U(1)

For the last example of the Z_2 grading formula we take the superalgebra analog of SU($n+1$)/U(n). Again we adopt the Gell-Mann notation with Hermitian generators F_i, $i = 1,2,\dots,(n+1)^2 - 1$. The a-number-valued generators $F_{n^2},\dots,F_{(n+1)^2-2}$ are combined into an n-component spinor K and the (imaginary) coset parameters are used to form a spinor γ in the same way that they were in the example of Sec. IIIB [see (19)]. By defining

$$\Gamma = i(F_{n^2}\gamma_{n^2} + \cdots + F_{(n+1)^2-2}\gamma_{(n+1)^2-2}),$$

we ensure that

$$\Gamma = i(\bar K\gamma + \bar\gamma K)/2. \tag{18}$$

The analog of the matrix operator J is given by

$$J_{\mathrm{SU}(n/1)} = -\sum_{i=1}^{n^2-1}\lambda_i F_i - (2(n-1)/n)^{1/2}F_{n(n+2)}I_n, \tag{35}$$

where λ_i is again the ith Gell-Mann matrix for SU(n). The algebra SU(n/1) may be summarized by Eqs. (21) and the multiple commutators are exactly those given in Eqs. (22) and (23). Because of this, the expression for the product of two coset transformations is given in Eq. (24).

In example IIIB it was stated that the calculations were easier to perform if instead of the Gell-Mann generators, the matrix generators were used. The same comments apply in this case where the $T_{\alpha\beta}$ satisfy[7]

$$[T_{\alpha\beta},T_{\gamma\delta}] = \delta_{\gamma\beta}T_{\alpha\delta} - \begin{bmatrix}\alpha\gamma\\ \beta\delta\end{bmatrix}\delta_{\alpha\delta}T_{\gamma\beta}; \tag{36}$$

here the Greek indices run from 1 to $n+1$ and

$$\begin{bmatrix}\alpha\gamma\\ \beta\delta\end{bmatrix} = (-1)^{((\alpha)+(\gamma))((\beta)+(\delta))}, \tag{37}$$

with

$$(\alpha) = \begin{cases} 0 & \text{for } 1 \leqslant \alpha \leqslant n, \\ 1 & \text{for } \alpha = n+1. \end{cases} \tag{38}$$

They also obey the constraints

$$(T_{\alpha\beta})^\dagger = T_{\beta\alpha} \quad \text{and} \quad \sum_{\alpha=1}^{n+1} T_{\alpha\alpha} = 0.$$

The generators of $SU(n)\times U(1)$ are identified as $J_{ij} = T_{ij}$ where $i,j = 1,2,...,n$. The coset generators are given by $L_i = T_{i,n+1}$ and $L_{i+n} = T_{n+1,i}$ and are a-number valued. The coset parameters are complex a-numbers and are such that $\eta_i^* = -\eta_{i+n}$. Then the calculations are simple and yield the result

$$\begin{aligned}\exp \Delta \exp \Gamma = {} & \exp\{\Delta + \Gamma + \tfrac{1}{4} i x^{-4}[(1 - 2x\cot(2x))(\eta_h \wedge \theta_h)(x^2\delta_{kl} + \eta_l \eta_k^*) \\ & + 4(x\cot(x) - 1)(x^2(\eta_k \wedge \theta_l) - (\eta_h \wedge \theta_h)\eta_k^* \eta_l)](\eta_k L_l + \eta_l^* L_k^\dagger)\} \\ & \times \exp\{\tfrac{1}{2} x^{-3}[(\eta_h \wedge \theta_h)\eta_i \eta_j^*(2\tan(x/2) - \tan(x)) + 2x^2(\eta_j \wedge \theta_i)\tan(x/2)] \\ & \times (J_{ij} + \delta_{ij} T_{n+1,n+1})\}.\end{aligned} \tag{39}$$

Again $\Gamma = i\mathbf{L}\cdot\eta$, $\Delta = i\mathbf{L}\cdot\boldsymbol{\theta}$, and $(\theta_j \wedge \eta_i)$ and x^2 are defined in (28) and (29), respectively. The indices h to l run from 1 to n with summation over repeated indices. Relevant details of the calculation using the matrix generators and the conversion between the two forms of the answer are given in the Appendix. Note that for $SU(n/1)/SU(n)\times U(1)$, both x^2 and y^2 are nilpotent c-numbers.

The examples of S^2, S^3, CP^2, and $OSp(1/4)/Sp(4)$ have already been performed by Delbourgo and Jarvis[3] and provide a useful check of our results. In each case the agreement is perfect.

In the general case it must be realized that the left-hand side of (3) does not involve the most general coset actions. Using the case of a Z_3 graded algebra, for example, we would have

$$\exp(i\delta_1 J_1)\exp(i\delta_2 J_2)\exp(i\gamma_1 J_1)\exp(i\gamma_2 J_2)$$

as the most general product of two coset actions. This problem has not, as yet, been fully solved and we are obliged to leave it for future study.

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APPENDIX

As has been stated in the text, it is considerably easier to do the $SU(n+1)/U(n)$ and $SU(n/1)/SU(n)\times U(1)$ calculations using the matrix generators rather than the Gell-Mann ones. The purpose of this Appendix is to repeat the above examples, this time treating them in the same way as $O(n)/O(n-1)$. Relevant details of the conversion between the expressions given in (27) and (39) with that in (24) are also presented.

1. SU($n+1$)/U(n)

Recall that the matrix generators satisfy

$$[T_{\alpha\beta}, T_{\gamma\delta}] = \delta_{\gamma\beta} T_{\alpha\delta} - \delta_{\alpha\delta} T_{\gamma\beta}, \tag{A1}$$

for $\alpha,\beta,\gamma,\delta = 1,2,...,n+1$. The T's are split into two groupings: $J_{ij} = T_{ij}$, where $i,j = 1,2,...,n$, and $L_i = T_{i,n+1}$, $L_{i+n} = T_{n+1,i}$. The Hermiticity property of the T's,

$$(T_{\alpha\beta})^\dagger = T_{\beta\alpha}, \tag{A2}$$

means that the coset parameters $\eta_1,...,\eta_{2n}$ are complex with

$$\eta_i^* = \eta_{i+n}, \tag{A3}$$

so that

$$\begin{aligned}\Gamma = i\mathbf{L}\cdot\boldsymbol{\eta} = i(& L_1\eta_1 + L_2\eta_2 + \cdots \\ & + L_n\eta_n + L_1^\dagger \eta_1^* + \cdots + L_n^\dagger L_n^*).\end{aligned}$$

With this notation, the $SU(n+1)$ algebra can be expressed as

$$[\Delta,\Gamma]_1 = (\theta_j \wedge \eta_i)(J_{ij} - \delta_{ij} T_{n+1,n+1}), \tag{A4a}$$

$$[J_{ij} - \delta_{ij} T_{n+1,n+1}, \Gamma] = i(\delta_{kj}\delta_{il} + \delta_{ij}\delta_{kl})(\eta_k L_l - \eta_l^* L_k^\dagger), \tag{A4b}$$

$$\begin{aligned}&[\eta_k L_l - \eta_l^* L_k^\dagger, \Gamma] \\ &\quad = i(\eta_i \eta_l^* \delta_{kj} + \eta_k \eta_j^* \delta_{il})(J_{ij} - -\delta_{ij} T_{n+1,n+1}),\end{aligned} \tag{A4c}$$

where $T_{n+1,n+1} = -\Sigma_{i=1}^n T_{ii}$ and $(\theta_j \wedge \eta_i)$ is given in (28). The multiple commutators are trivially found to be [with x^2 given in (29)]

$$[\Delta,\Gamma]_{2m+1} = (-1)^{m+1}((4^m - 1)(\eta_h \wedge \theta_h)\eta_i \eta_j^* x^{2m-2} + (\eta_j \wedge \theta_i)x^{2m})(J_{ij} - \delta_{ij} T_{n+1,n+1}), \tag{A5a}$$

$$\begin{aligned}[\Delta,\Gamma]_{2m} = i(-1)^m\{ & [(\eta_k \wedge \theta_l) + 4^{m-1}(\eta_h \wedge \theta_h)\delta_{kl}]x^{2m-2} \\ & + (4^{m-1} - 1)(\eta_h \wedge \theta_h)\eta_k^* \eta_l x^{2m-4}\}(\eta_k L_l - \eta_l^* L_k^\dagger), \quad m \geqslant 1,\end{aligned} \tag{A5b}$$

and these expressions yield (27).

The task of converting (27) into (24) is quite easy if one realizes that (for $i = 1,2,...,n$.)

$$2\eta_i = \gamma_i, \tag{A6a}$$

$$2\eta_{i+n} = \bar{\gamma}_i, \tag{A6b}$$

$$L_i = \bar{K}_i, \tag{A7a}$$

$$L_{i+n} = K_i, \tag{A7b}$$

where, for example, γ_i denotes the ith component of the spinor γ; see (19). The following equalities are then established:

$$4x^2 = y^2, \tag{A8}$$

$$4(\eta_i \wedge \theta_i) = (\bar{\gamma}\delta - \bar{\delta}\gamma), \tag{A9}$$

$$4(\theta_j \wedge \eta_i)(J_{ij} - \delta_{ij} T_{n+1,n+1}) = \bar{\delta} J_{\mathrm{SU}(n+1)}\gamma - \bar{\gamma} J_{\mathrm{SU}(n+1)}\delta, \tag{A10}$$

$$4\eta_j^* \eta_i (J_{ij} - \delta_{ij} T_{n+1,n+1}) = \bar{\gamma} J \gamma, \tag{A11}$$

$$2(\eta_k L_k - \eta_k^* L_k^\dagger) = (\bar{K}\gamma - \bar{\gamma} K), \tag{A12}$$

$$16i(\eta_k \wedge \theta_l)(\eta_k L_l - \eta_l^* L_k^\dagger) = 4y^2 \Delta - 2(\bar{\gamma}\delta + \bar{\delta}\gamma)\Gamma - i(\bar{\delta}\gamma - \bar{\gamma}\delta)(\bar{K}\gamma - \bar{\gamma}K), \tag{A13}$$

$$8\eta_k^* \eta_l (\eta_k L_l - \eta_l^* L_k^\dagger) = y^2(\bar{K}\gamma - \bar{\gamma}K), \tag{A14}$$

where

$$\Gamma = i\mathbf{L}\cdot\boldsymbol{\eta} = \tfrac{1}{2}i(\bar{K}\gamma + \bar{\gamma}K), \tag{A15}$$

$$\Delta = i\mathbf{L}\cdot\boldsymbol{\theta} = \tfrac{1}{2}i(\bar{K}\delta + \bar{\delta}K). \tag{A16}$$

The reader may verify that insertion of (A8)–(A16) in (27) gives (24).

2. SU(n/1)/SU(n)×U(1)

In this example, the matrix generators $T_{\alpha\beta}$ satisfy

$$[T_{\alpha\beta}, T_{\gamma\delta}] = \delta_{\gamma\beta} T_{\alpha\delta} - \begin{bmatrix}\alpha\gamma\\ \beta\delta\end{bmatrix} \delta_{\alpha\delta} T_{\gamma\beta}, \tag{A17}$$

where $\alpha, \beta, \gamma, \delta = 1,2,...,n+1$, and $\left[\begin{smallmatrix}\alpha\gamma\\ \beta\delta\end{smallmatrix}\right]$ is defined in (37). Again we have $J_{ij} = T_{ij}$, $L_i = T_{i,n+1}$, and $L_{i+n} = T_{n+1,i}$, where $i,j = 1,2,...,n$; however, the L's are now a-number generators. Equation (A2) holds but because the coset parameters are a-numbers, they obey

$$\eta_i^* = -\eta_{i+n}. \tag{A18}$$

Defining $\Gamma = i\mathbf{L}\cdot\boldsymbol{\eta}$ ensures that (A15) is still true. The SU(n/1) algebra is given by

$$[\Delta, \Gamma]_1 = -(\theta_j \wedge \eta_i)(J_{ij} + \delta_{ij} T_{n+1,n+1}), \tag{A19a}$$

$$[J_{ij} + \delta_{ij} T_{n+1,n+1}, \Gamma] = -i(\delta_{jk}\delta_{il} - \delta_{ij}\delta_{kl})(\eta_k L_l + \eta_l^* L_k^\dagger), \tag{A19b}$$

$$[\eta_k L_l + \eta_l^* L_k^\dagger, \Gamma] = -i(\delta_{jk}\eta_i\eta_l^* + \delta_{il}\eta_k\eta_j^*) \times (J_{ij} + \delta_{ij} T_{n+1,n+1}). \tag{A19c}$$

Again $T_{n+1,n+1} = -\Sigma_{i=1}^n J_{ii}$ and $(\theta_j \wedge \eta_i)$ is given in (28). The multiple commutators are readily evaluated;

$$[\Delta, \Gamma]_{2m+1} = (-1)^{m+1}\{(4^m - 1)(\eta_h \wedge \theta_h)\eta_i \eta_j^* x^{2m-2} - (\eta_j \wedge \theta_i) x^{2m}\}(J_{ij} + \delta_{ij} T_{n+1,n+1}), \tag{A20a}$$

$$[\Delta, \Gamma]_{2m} = i(-1)^m\{[(\eta_k \wedge \theta_l) - 4^{m-1}(\eta_h \wedge \theta_h)\delta_{kl}] x^{2m-2} + (4^{m-1} - 1)(\eta_h \wedge \theta_h)\eta_k^* \eta_l x^{2m-4}\} \times (\eta_k L_l + \eta_l^* L_k^\dagger), \quad m \geqslant 1, \tag{A20b}$$

with x^2 defined in (29). Inserting these expressions into (13) leads directly to (39).

The analog of (A6b) is

$$2\eta_{i+n} = -\bar{\gamma}_i, \tag{A6b$'$}$$

with the (–) sign occurring because the elements of the spinor γ are purely imaginary. Equations (A6a) and (A7) remain unaltered, as do (A8), (A9), (A15), and (A16), while (A10)–(A14) become[8]

$$-4(\theta_j \wedge \eta_i)(J_{ij} + \delta_{ij} T_{n+1,n+1}) = \bar{\delta} J_{\mathrm{SU}(n/1)}\gamma - \bar{\gamma} J_{\mathrm{SU}(n/1)}\delta, \tag{A10$'$}$$

$$-4\eta_j^* \eta_i (J_{ij} + \delta_{ij} T_{n+1,n+1}) = \bar{\gamma} J \gamma, \tag{A11$'$}$$

$$2(\eta_k L_k + \eta_k^* L_k^\dagger) = (\bar{\gamma}K - \bar{K}\gamma), \tag{A12$'$}$$

$$16i(\eta_k \wedge \theta_l)(\eta_k L_l + \eta_l^* L_k^\dagger) = 4y^2\Delta - 2(\bar{\delta}\gamma + \bar{\gamma}\delta)\Gamma - i(\bar{\delta}\gamma - \bar{\gamma}\delta)(\bar{K}\gamma - \bar{\gamma}K), \tag{A13$'$}$$

$$8\eta_k^* \eta_l (\eta_k L_l + \eta_l^* L_k^\dagger) = y^2(\bar{K}\gamma - \bar{\gamma}K). \tag{A14$'$}$$

If these expressions are inserted in (39), one obtains (24).

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[4]This means that the coset space parameters are strictly associated with those generators of the algebra that do not form the subalgebra.

[5]See, e.g., W. Witschel, J. Phys. A **8**, 143 (1975).

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[8]We normalize the λ matrices of SU(n/1) so that

$$\operatorname{trace}(\lambda_i\lambda_j) = \begin{cases} 0, & i \neq j, \\ 2, & i = j = 1,2,...,(n+1)^2 - 2, \end{cases}$$

$$\operatorname{supertrace}(\lambda^2_{n(n+2)}) = -2.$$

A duality consistent phase convention for complex conjugation in SUn

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We have argued that a simple phase convention for all involutive mappings can be chosen so the algebra of inner product couplings in SUn is identical to that for outer products in S_L. Pure real phases with a single ± 1 entry in any row or column can represent the permutation matrix for transposition in order of the two component irreducible representations (irreps) in a binary coupling, the matrix for association in S_L with respect to the alternating group A_L, the Derome–Sharp matrix, and the $1jm$ factor. The latter two are required by complex conjugation in SUn. In our previous work, we have proposed specific prescriptions for assigning the phase under transposition and association and have shown them to be consistent with duality. In this work, we propose a duality consistent prescription for assigning the phase of the Derome–Sharp matrix and thus of the $1jm$ factor which is related to it by association.

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I. PHASE AND DUALITY

In our previous work (I),[1] we have considered the symmetry properties required of phase conventions for the coupling algebra of the unitary unimodular group SUn to be consistent through duality with coupling in the symmetric group S_L. For a more explicit description of the notation and terminology, and citation of past works on this subject the reader is referred to I. Our work has concentrated on the duality of outer product coupling in S_L/S_{L_j} with inner product coupling in SUn, although an analogous duality holds for inner product coupling in S_L and outer product coupling in SUnm/SUnSUm.[2] Phase conventions must be prescribed for transposition in the order of the component irreps in a binary coupling $(\lambda{:}\lambda_1\lambda_2)\leftrightarrow(\lambda{:}\lambda_2\lambda_1)$, association in S_L with respect to the alternating group A_L $(\tilde{\lambda}{:}\tilde{\lambda}_1\tilde{\lambda}_2)$, complex conjugation in SUn requiring the Derome–Sharp factor[3] $([l^n/\lambda]{:}[l_1^n/\lambda_1]\,[l_2^n/\lambda_2])$, and complex conjugation in a basis adapted to SUn/SUn_1SUn_2 requiring the $1jm$ factor $([l^n/\lambda]{:}[l^{n_1}/\lambda_1]\,[l^{n_2}/\lambda_2])$, where $n=n_1+n_2$. These conventions are all interrelated by duality. In I, the symmetries these phase conventions must exhibit to be consistent with duality are specified and a detailed examination of the role of multiplicity in outer product coupling in S_L is made. We have argued that a set of phase conventions consistent with duality can be chosen so each of the above factors is in real pure phase form (a single ± 1 in any row or column of a phase matrix with rows and columns labeled by the multiplicities). These pure phase conventions remain consistent, although modified, upon introducing symmetrized products appropriate to S_{2L}/S_L wreath S_2. In addition, we have proposed specific conventions assigning the phase sign under transposition and under association, and have shown them to satisfy all the requirements of duality. The conventions for the Derome–Sharp factor and the $1jm$ factor have been shown to be related by association. Although the Derome–Sharp factor can almost always be chosen to be the trivial positive unit $(+1)$ factor, we have shown there are some couplings in which this factor must be negative in order to maintain reality of the coupling coefficients as implied by choosing real matrix representations of S_L. However, we offered no convention for fixing the Derome–Sharp factor and/or the $1jm$ factor, considering this an unresolved question.

In this work we propose a prescription for fixing the Derome–Sharp factor almost always as the trivial positive unit, but in most cases where symmetric and antisymmetric products of S_{2L}/S_L wr S_2 separate multiplicities, we must choose a negative sign for the antisymmetrized coupling. This sign is required for the same reason it comes about in bringing the transposition phase to diagonal form. Fixing the Derome–Sharp factor fixes the $1jm$ factor by association. Indeed, when the Derome–Sharp factor is the trivial positive unit, the $1jm$ factor is the association sign for the double coset matrix element specifying the $1jm$ factor. We carry out this prescription for the $1jm$ factor in the Gel'fand scheme SUn/SU$n-1$ and show it reduces to the usual convention for SU2.

II. DOUBLE COSET FORMS

The Derome–Sharp factor is a phase matrix which must be considered when relating the coupling coefficient for a triad to that for the complex conjugate triad in a given group. It can be related to a particular $9j$ recoupling coefficient involving three scalar entries. For SUn as shown in I, it can be identified with the double coset matrix element (DCME):

$$A\,(n\lambda{:}\lambda_1\lambda_2)rr^* \equiv \left(\frac{\langle\lambda_1\rangle_n\langle\lambda_2\rangle_n}{\langle\lambda\rangle_n}\right)^{1/2} \times \begin{bmatrix} [(l_1+l_2)^n] & [l_1^n] & [l_2^n] \\ \lambda & \lambda_1 & \lambda_2 \\ \left[\dfrac{(l_1+l_2)^n}{\lambda}\right] & \left[\dfrac{l_1^n}{\lambda_1}\right] & \left[\dfrac{l_2^n}{\lambda_2}\right] \end{bmatrix}_{r^*}^{r}. \quad (2.1)$$

In this paper, we will consider the Derome–Sharp factor as identical to the DCME, ignoring the magnitude factor since it is only the multiplicity resolution (rr^*) and the sign which concern us here. Using the transposition phase proposed in I, we have the following equalities:

$$
\begin{aligned}
A\,(n\lambda{:}\lambda_1\lambda_2)rr^* &= A\,(n\lambda{:}\lambda_2\lambda_1)ss^* \\
&= A\,(n\lambda^*{:}\lambda_1^*\lambda_2^*)r^*r \\
&= A\,(n\lambda^*{:}\lambda_2^*\lambda_1^*)s^*s.
\end{aligned} \tag{2.2}
$$

That is, the operations of transposition and complex conjugation commute and the Derome–Sharp factor does not change sign under either of these operations. It is also immaterial if one considers the triad in the vector coupling form $(\lambda{:}\lambda_1\lambda_2)r$ or the more symmetric $3j$ form $([l^n]{:}\lambda_1\lambda_2\lambda_3)r$, where $\lambda\equiv[l^n/\lambda_3]$ because $A\,(n\lambda{:}\lambda_1\lambda_2)rr^* = \mathrm{A}([l^n]{:}\lambda_1\lambda_2\lambda_3)rr^*$.

The $1jm$ factor is a phase matrix which must be considered when coupling an irrep in a basis adapted to a specific subgroup sequence with its complex conjugate irrep to form a scalar. It has the form of an isoscalar factor. For a basis adapted to $\mathrm{SU}n_1+n_2/\mathrm{SU}n_1\mathrm{SU}n_2$ as shown in I, it can be identified with a weighted double coset matrix element (WDCME):

$$
((n_1+n_2)\lambda{:}n_1\lambda_1 n_2\lambda_2) = \left(\frac{\langle\lambda\rangle_{(n_1+n_2)}}{\langle\lambda_1\rangle_{n_1}\langle\lambda_2\rangle_{n_2}}\right)^{1/2}
\times\begin{pmatrix} [l^{n_1+n_2}] & [l^{n_1}] & [l^{n_2}] \\ \lambda & \lambda_1 & \lambda_2 \\ \left[\dfrac{l^{n_1+n_2}}{\lambda}\right] & \left[\dfrac{l^{n_1}}{\lambda_1}\right] & \left[\dfrac{\lambda^{n_2}}{\lambda_2}\right] \end{pmatrix}\begin{matrix} r \\ \\ \bar r \end{matrix}. \tag{2.3}
$$

Analogously, we will consider the $1jm$ factor as identical to the WDCME and, equivalently, to the DCME of the same form, ignoring the magnitude factors since it is the multiplicity resolution $(r\bar r)$ and the sign which concern us here. Transposition of the rows gives

$$
\begin{aligned}
((n_1+n_2)\lambda{:}n_1\lambda_1 n_2\lambda_2)r\bar r &= (-1)^{L_1n_2+L_2n_1} \\
&\quad\times\left((n_1+n_2)\left[\frac{l^{(n_1+n_2)}}{\lambda}\right]{:}n_1\left[\frac{l^{n_1}}{\lambda_1}\right]n_2\left[\frac{l^{n_2}}{\lambda_2}\right]\right)
\end{aligned} \tag{2.4}
$$

as required by consideration of Schur's invariant in $\mathrm{SU}n_1+n_2/\mathrm{SU}n_1 SUn_2$. An analogous relation by transposition of the columns can be given but it adds nothing to the development here.

In I it was noted that the form of the Derome–Sharp factor is associate to that of the $1jm$ factor, so these phase matrices are related by the duality operation of association in S_L.

$$
\begin{aligned}
&\begin{bmatrix} [(l_1+l_2)^n] & [l_1^n] & [l_2^n] \\ \lambda & \lambda_1 & \lambda_2 \\ \left[\dfrac{(l_1+l_2)^n}{\lambda}\right] & \left[\dfrac{l_1^n}{\lambda_1}\right] & \left[\dfrac{l_2^n}{\lambda_2}\right] \end{bmatrix}\begin{matrix} r \\ \\ r^* \end{matrix} = (-1)^{L_2(nl_1-L_1)}([(l_1+l_2)^n]{:}[l_1^n][l_2^n])\left([(l_1+l_2)^n]{:}\lambda\left[\frac{(l_1+l_2)^n}{\lambda}\right]\right) \\
&\quad\times\left([l_1^n]{:}\lambda_1\left[\frac{l_1^n}{\lambda_1}\right]\right)\left([l_2^n]{:}\lambda_2\left[\frac{l_2^n}{\lambda_2}\right]\right)(\lambda{:}\lambda_1\lambda_2)_{r\tilde r}\left(\left[\frac{(l_1+l_2)^n}{\lambda}\right]{:}\left[\frac{l_1^n}{\lambda_1}\right]\left[\frac{l_2^n}{\lambda_2}\right]\right)_{r^*\tilde r^*}\begin{bmatrix} [n^{l_1+l_2}] & [n^{l_1}] & [n^{l_2}] \\ \tilde\lambda & \tilde\lambda_1 & \tilde\lambda_2 \\ \left[\dfrac{n^{l_1+l_2}}{\tilde\lambda}\right] & \left[\dfrac{n^{l_1}}{\tilde\lambda_1}\right] & \left[\dfrac{n^{l_2}}{\tilde\lambda_2}\right] \end{bmatrix}\begin{matrix} \tilde r \\ \\ \bar{\tilde r} \end{matrix},
\end{aligned} \tag{2.5}
$$

where $\bar{\tilde r} = \tilde r^*$. The six factors on the lhs are association phases which may be evaluated according to the prescription given in I (Eq. 7.5). Thus fixing a phase convention for either the Derome–Sharp factor or the $1jm$ factor fixes the convention for the other. In I it was noted that the Derome–Sharp factor usually can be chosen as the trivial positive unit phase, but there are exceptions when duality requires the negative assignment. The first negative example given is $A\,(3[3,2,1]{:}[2,1]\otimes[1^2]) = -1$. Here we will argue that the Derome–Sharp factor in unsymmetrized products can always be chosen as $+1$, and in symmetrized products it may be chosen as $+1$ except in those cases where $(\lambda{:}\lambda_1\lambda_2)\simeq([(l_1+l_2)^n/\lambda]{:}[l_1^n/\lambda_1][l_2^n/\lambda_2])$, $\lambda_1\simeq\lambda_2$ and use of the symmetrized and antisymmetrized products separate the multiplicity in which case it must be chosen as $A\,(n\lambda{:}\lambda_1\otimes\sigma)=\phi_\sigma$, where $\phi_\sigma = \pm 1$ as $\sigma=[2]$ or $[1^2]$. The $1jm$ factor sign is fixed by association and is consistent with duality and the Schur classification of irreps.

III. THE DEROME–SHARP FACTOR PHASE

In I we characterized a triad coupling by a set of positive integers $m_{ij}(k)$ specifying the number of nodes transferred from row i of component irrep λ_k to the jth row of the composite irrep built on $\lambda_{k'}$ in the ith step of carrying out the Littlewood Richardson rules for outer products in S_L/S_{L_j}. Thus we have the transcription

$$
\begin{aligned}
(\lambda{:}\lambda_1\lambda_2)r &\equiv ([l_i]{:}[l(1)_i][l(2)_i])r \\
&= \left(\left[\sum_j m(1)_{ij} + \sum_h m(2)_{hi}\right]{:}\left[\sum_j m(1)_{ij}\right]\left[\sum_j m(2)_{ij}\right]\right).
\end{aligned} \tag{3.1}
$$

Prescriptions were given for determining the sign of the transposition phase and the association phase from the set $\{m_{ij}(k)\}$. It was also noted that there was a natural mapping under complex conjugation giving

$$
m(k')^*_{ij} = m(k)_{(n-j+1)(n-i+1)} + \delta_{ij}(l(k')_i - l_{n-i+1}). \tag{3.2}
$$

Here we correct an error in the delta factor of Eq. (7.13) of I which does not affect the arguments of that paper. Relation (3.2) specifies the multiplicity mapping under complex conjugation and transposition. For $\lambda_1\simeq\lambda_2$, the transposition phase matrix is real and symmetric. The phase prescription for transposition proposed in I results in a real phase form which is a sign independent of the multiplicity times a permutation matrix which can be ordered to have either the unit or two by two block matrix $\binom{0\ 1}{1\ 0}$ along the diagonal. The transposition phase matrix is diagonalized in the multiplicity by transforming to symmetrized products. Let $r(\sigma)\equiv|\lambda{:}\lambda_1\otimes[\sigma]|$, then character theory of S_L requires the character of the class (2^{L_1}) in $\lambda\vdash 2L_1$ to be

$$[\lambda](2^{L_1}) = \sum_{\lambda_1\vdash L_1} |\lambda_1|(r(2) - r(1^2)). \qquad (3.3)$$

Thus the transposition phase matrix in its nondiagonal but real phase form has $|r(2) - r(1^2)|$ units on the diagonal, and minimum $(r(\sigma))$ two by two $\binom{0\ 1}{1\ 0}$ blocks on the rest of the diagonal.

For

$$(\lambda{:}\lambda_1\lambda_2)\simeq\left(\left[\frac{(l(1)+l(2))^n}{\lambda}\right]{:}\left[\frac{l(1)^n}{\lambda_1}\right]\left[\frac{l(2)^n}{\lambda_2}\right]\right),$$

the Derome–Sharp factor also has a symmetric real phase form. If, in addition, $\lambda_1\simeq\lambda_2$, then the mapping Eq. (3.2) also is represented by a real symmetric phase matrix. Since both of these matrices commute with the transpose phase matrix, they must both have a block diagonal form similar to that discussed above. The number of two by two blocks may be different, but the reduction is such that one has submatrix multiplication

$$\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}=\begin{pmatrix}1&0\\0&1\end{pmatrix} \quad\text{or}\quad \begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1&0\\0&1\end{pmatrix}=\begin{pmatrix}0&1\\1&0\end{pmatrix}.$$

That is, in the natural permutation representation of the symmetric group on the multiplicity space $S_{r(2)+r(1^2)}$, these phase matrices belong to commuting elements of the two fold classes $(1^{(r(2)+r(1^2)-2p)}2^p)$.

As pointed out in I, the only case in which there might be an inconsistency between duality and assuming real phase form is when, in addition, one has triad equivalence under association, i.e., $(\lambda{:}\lambda_1\lambda_2)\simeq(\tilde{\lambda}{:}\tilde{\lambda}_1\tilde{\lambda}_2)$. The simultaneous application of all three triad equivalences restricts the form of the irreps to two types which are given in Table 6.1 of I. For these types, we show, in the Appendix, that the relation Eq. (3.2) is the identity mapping and thus the Derome–Sharp factor must be identified except for overall sign with the tranposition matrix. Diagonalizing the transposition phase matrix by transforming to symmetrized products requires the negative assignment to the corresponding Derome–Sharp factor phase for each two by two block $\binom{0\ 1}{1\ 0}\to\binom{1\ \ 0}{0\ -1}$. For example, the characteristic triads for the two types are

$$\Phi([3,2,1]{:}[2,1]^2) = \begin{pmatrix}0&1\\1&0\end{pmatrix} = \mathrm{A}(3[3,2,1]{:}[2,1]^2)\mapsto\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

with

$$\Phi([3,2,1]{:}[2,1]\otimes[1^2]) = -1 = A(3[3,2,1]{:}[2,1]\otimes[1^2])$$

and

$$\Phi([4^2,2^2]{:}[3,2,1]^2) = \begin{pmatrix}1&0\\0&1\end{pmatrix} = A(4[4^2,2^2]{:}[3,2,1]^2)$$

which remains invariant under transformation to symmetrized products [i.e., $r(2)=2$ and $r(1^2)=0$]. If the associate triads are not equivalent, there is no question that real phase form is consistent with duality, but the matrix representing Eq. (3.2) is no longer the identity. The multiplicity labeling for each triad

$$(\lambda{:}\lambda_1^2) = \left(\left[\frac{(2l(1)_1)^n}{\lambda}\right]{:}\left[\frac{l(1)_1^n}{\lambda_1}\right]^2\right)$$

can be used to determine the form of the matrix representing Eq. (3.2), while character theory establishes the form of the transpose phase matrix. The product of these two matrices gives the Derome–Sharp matrix. The transformation of each two by two block $\binom{0\ 1}{1\ 0}$ of the Derome–Sharp matrix to diagonal form using symmetrized products requires negative assignments for those $A(\lambda{:}\lambda_1\otimes[1^2])$. However, those portions of the Derome–Sharp factor which were already diagonal but correspond to a $\binom{0\ 1}{1\ 0}$ block in the transposition phase remain diagonal on transformation to symmetrized products with positive phase assigned to both components. For example $|[6,5,3,2]\ [4,3,1]^2| = 5$ with $r(2)=2$ and $r(1^2)=3$, the $(i\neq j)$ sets m_{ij} labeling the unsymmetrized multiplicities are

$$m_{12}=m_{13}=m_{23}=m_{24}=m_{34}=1,$$
$$m_{12}=m_{14}=m_{34}=1,\quad m_{23}=2,$$
$$m_{13}=m_{14}=m_{24}=1,$$
$$m_{12}=m_{13}=1,\quad m_{24}=2,$$
$$m_{13}=2,\quad m_{24}=m_{34}=1,$$

for which Eq. (3.2) has representation matrix

$$\begin{pmatrix}1&0&0&0&0\\0&1&0&0&0\\0&0&1&0&0\\0&0&0&0&1\\0&0&0&1&0\end{pmatrix}.$$

The transpose matrix must have the nondiagonal form

$$\Phi([6,5,3,2]{:}[4,3,1]^2) = -\begin{pmatrix}1&0&0&0&0\\0&0&1&0&0\\0&1&0&0&0\\0&0&0&0&1\\0&0&0&1&0\end{pmatrix}.$$

Thus

$$A(4[6,5,3,2]{:}[4,3,1]^2) = \begin{pmatrix}1&0&0&0&0\\0&0&1&0&0\\0&1&0&0&0\\0&0&0&1&0\\0&0&0&0&1\end{pmatrix},$$

which transforms, using symmetrized products, to

$$A([6,5,3,2]{:}[4,3,1]\otimes\sigma) = \begin{pmatrix}1&0&0&0&0\\0&1&0&0&0\\0&0&-1&0&0\\0&0&0&1&0\\0&0&0&0&1\end{pmatrix}.$$

In summary, a phase convention consistent with duality may choose the Derome–Sharp factor as the trivial (positive) unit except for symmetrized products of the form $(\lambda{:}\lambda_1\otimes[1^2])$. Even in these latter cases, a negative assignment need be made only when it results from diagonalizing the two by two block $\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$ in the nondiagonal real phase form of the Derome–Sharp matrix. The occurrence of the nondiagonal two by two blocks is determined by the forms of the matrix representing Eq. (3.2) and the matrix representing the transpose phase matrix as fixed by character theory in S_L.

IV. THE 1*jm* FACTOR

Establishing a convention for the Derome–Sharp matrix fixes the 1*jm* factor by the association relation (2.5) which follows from duality. The association phases may be evaluated by the convention given in Eq. (7.5) of I. This, together with the mapping (3.2), allows the 1*jm* factor to be calculated in a straightforward but tedious manner. In the general case, we have been unable to find any algorithm simplifying the 1*jm* phase calculation.

For the Gel'fand and canonical basis SUn/SU$n-1$ the 1*jm* factor has the association sign of the DCME

$$\begin{bmatrix} [l^n] & [l^{n-1}] & [l] \\ [l_i] & [l_i - m_i] & [\Sigma m_i] \\ [l - l_{n-i+1}] & [l - l_{n-i} + m_{n-i}] & [\Sigma(l_{n-i} - l_{n-i+1} - m_{n-i})] \end{bmatrix},$$

where $1 \leqslant i \leqslant n-1$ and $l_1 = l$ and $l_n = 0$. For this subgroup adaption, the 1*jm* factor simplifies to

$$(n\lambda{:}(n-1)[l_i - m_i]) = (-1)\sum_i m_{n-2i+1}. \qquad (4.1)$$

That is, for SU2 the 1*jm* phase is $(-1)^{m_1}$. Using $j = l/2$, $m = l/2 - m_1$ gives $(-1)^{m_1} = (-1)^{j-m}$ as usual. For SU_3/SU_2 the 1*jm* phase factor is $(-1)^{m_2}$, for SU_4/SU_3 the 1*jm* phase factor is $(-1)^{m_1+m_3}$, etc.

APPENDIX

For $\lambda_1 \simeq \lambda_2$ and $(\lambda{:}\lambda_1^2) \simeq ([(2l)^n/\lambda]{:}[l^n/\lambda_1]^2) \simeq (\tilde\lambda{:}\tilde\lambda_1^2)$, we wish to show the mapping Eq. (3.2).

$$m_{ij} \Rightarrow m_{(n-j+1)(n-i+1)} + \delta_{ij}(l - l_{n-i+1})$$

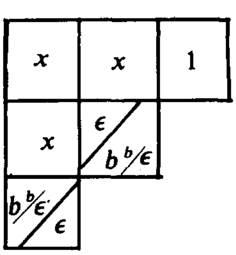
is the identity. The set of triad equivalences are satisfied only for triads of the form [I, Eq. (6.18) and Table 6.1]

$$([(3b)^b,(2b)^b,b^b]{:}[(2b)^b,b^b]^2)$$

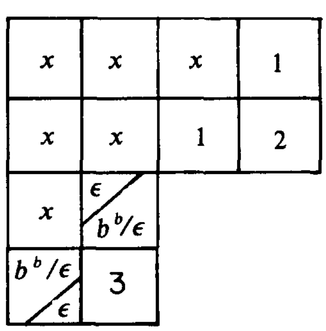
or

$$([(4b)^{2b},(2b)^{2b}]{:}[(3b)^b,(2b)^b,b^b]^2)$$

for which $l = 2b$, $n = 3b$; or $l = 3b$, $n = 4b$, respectively. Consideration of the Littlewood–Richardson rules for outer products in S_L shows the coupling can be represented schematically in terms of $[b^b]$ blocks as



or



where the multiplicity is in one to one correspondence with all irreps ϵ such that $|[b^b]{:}\epsilon[b^b/\epsilon]| = 1$. The explicit correspondence is, with $1 \leqslant k, k' \leqslant b$,

$$\begin{aligned}
m_{k,k'} &= \delta_{kk'} b \quad \text{or} \\
&= m_{k,k'} = m_{k,b+k'} = m_{2b+k,3b+k}, \\
m_{k,b+k} &= \delta_{kk'} \epsilon_k \quad \text{or} \\
&= m_{k,2b+k'}, \\
m_{k,2b+k'} &= \epsilon_{k-k'} - \epsilon_{k-k'+1} \quad (k \geqslant k') \quad \text{or} \\
&= m_{k,3b+k'}, \\
m_{b+k,b+k'} &= \epsilon_{k'-k} - \epsilon_{k'-k+1} \quad (k' \geqslant k) \quad \text{or} \\
&= m_{b+k,2b+k'}, \\
m_{b+k,2b+k'} &= \delta_{kk'} \epsilon_{b-k+1} \quad \text{or} \\
&= m_{b+k,3b+k'},
\end{aligned}$$

respectively.

Use of (3.2) shows it to be the identity map for either type of triad. That is, for these types of triads, the mapping of multiplicities under complex conjugation is identical to the mapping under transposition of the component irreps.

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Eigenvalues of Casimir operators for the general linear and orthosymplectic Lie superalgebras

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A Racah basis is introduced for the generators of these matrix superalgebras and explicit formulas are derived for eigenvalues of Casimir operators in terms of the components of the highest weight. The result contains, as special cases, the corresponding expressions for the general linear, orthogonal, and symplectic Lie algebras.

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I. INTRODUCTION

Casimir operators for the classical Lie algebras have been studied by many authors. In particular, for representations possessing a highest-weight vector, eigenvalues of the Casimir operators have been calculated in terms of the components of the highest weight. The pioneering work along these lines was done by Perelomov and Popov,[1] by Louck and Biedenharn,[2] and by Okubo.[3] Particularly simple expressions, showing the similarity between the various classical Lie algebras, were obtained by Nwachuku and Rashid.[4]

The purpose of the present work is to extend the above results to the general linear and orthosymplectic Lie superalgebras. These are matrix algebras, just like the classical Lie algebras, and therefore a matrix notation can be conveniently used to label the generators. This basis for the generators will be called the Racah basis since it is a natural generalization of the basis proposed by Racah for the classical Lie algebras.[5] The detailed description of the Racah basis for the general linear and orthosymplectic Lie superalgebras is given in Sec. II, together with a definition of tensor operators and construction of invariants.

In Sec. III, the eigenvalue C_j of the jth degree Casimir operator is expressed in terms of the jth power of the Perelomov–Popov matrix. Up to this point, the various Lie superalgebras are treated simultaneously. It remains to diagonalize the Perelomov–Popov matrix. In Sec. IV, this is done in detail for the orthosymplectic superalgebras osp$(2m+1/2n)$; in Sec. V, for the orthosymplectic superalgebra osp$(2m/2n)$; and in Sec. VI, for the general linear superalgebra u(m/n).

The final result is remarkably simple, namely,

$$C_j = \sum_a [a](l_a)^j s_a \prod_{k\neq 0,a,\bar a}\left(1+\frac{[k]}{l_k-l_a}\right),$$

with

$$s_a = \begin{cases} 1 & \text{for u}(m/n) \\ 1+(1-\delta_{a0})\dfrac{[a]-(-)^p}{l_{\bar a}-l_a} & \text{for osp}(p/2n)\end{cases}$$

The notation is explained more fully in what follows; here we just want to mention that $[a]$ refers to the grading and l_a is the diagonal element of the Perelomov–Popov matrix and is given by a linear function of the ath component of the highest weight.

Some partial results on the subject of Casimir operators for superalgebras have been obtained previously. Bednar and Sachl[6a] consider osp$(1/2m)$ only, for which they give explicit formulas for the quadratic and quartic Casimir operators in terms of the generators, and outline a procedure for the operators of higher degree; they do not discuss the eigenvalues. Jarvis and Green[6b] consider the same superalgebras as we do (as well as the special linear superalgebra) and construct Casimir operators of arbitrary degree by means of tensor operators just as we do. They give explicit formulas for the eigenvalues in terms of highest weights in an arbitrary irreducible representation for the linear and quadratic Casimir operators of u(n/m) and osp$(n/2m)$. Our results are in exact agreement for these cases. Balantekin and Bars[6c] and Balantekin[6d] concentrate on the special linear superalgebra which we omit.

Most recently, while this work was being completed, a preprint appeared of a paper by Scheunert.[7] Our final formulas for the eigenvalues are identical. Scheunert's approach is more abstract using elegant mathematical language while our approach uses language common among physicists. In particular, we give a detailed description of the Racah basis for the generators and the diagonalization of the Perelomov–Popov matrix; while these topics are implicit in Scheunert's work, very few details are given.

II. THE RACAH BASIS AND TENSOR OPERATORS

The generators of the orthosymplectic Lie superalgebra osp$(2m+1/2n)$ are denoted in the Racah basis[5] by G^a_b with the indices ranging from $-(m+n)$ to $+(m+n)$, zero *included*. They obey the supercommutation relations

$$\begin{aligned}[][G^a_b, G^c_d\}\\ &= \delta^c_b\, G^a_d - (-)^{(\eta_a+\eta_b)(\eta_c+\eta_d)}\,\delta^a_d\, G^c_b \\ &\quad - \epsilon^{\bar a}\epsilon^b(-)^{\eta_a\eta_b}\left[\delta^c_{\bar a}\, G^{\bar b}_d - (-)^{(\eta_a+\eta_b)(\eta_c+\eta_d)}\,\delta^{\bar b}_d\, G^c_{\bar a}\right],\end{aligned} \tag{2.1}$$

where the supercommutator $[\ ,\ \}$ denotes

$$[G^a_b, G^c_d\} \equiv G^a_b\, G^c_d - (-)^{(\eta_a+\eta_b)(\eta_c+\eta_d)}\, G^c_d\, G^a_b \tag{2.2}$$

and

$$\bar a \equiv -a. \tag{2.3}$$

The η_a define the grading:

$$\eta_a = \begin{cases} 0 & \text{for } -m\leqslant a\leqslant +m, \\ 1 & \text{for } m+1\leqslant |a|\leqslant m+n,\end{cases} \tag{2.4}$$

and

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$$\epsilon^a = \begin{cases} 1 & \text{for } -m \leqslant a \leqslant m, \\ \operatorname{sgn} a & \text{for } m+1 \leqslant |a| \leqslant m+n. \end{cases} \tag{2.5}$$

Lastly these generators are antisymmetric in the sense

$$G^a_b = -\epsilon^{\bar a}\epsilon^b(-)^{\eta_a\eta_b}G^{\bar b}_{\bar a}. \tag{2.6}$$

Note that

$$\epsilon^a\epsilon^a = +1, \quad \epsilon^a\epsilon^{\bar a} = (-)^{\eta_a}. \tag{2.7}$$

The generators G^a_b are called even if $(-)^{\eta_a+\eta_b} = +1$, and odd if $(-)^{\eta_a+\eta_b} = -1$. It follows that the supercommutator of two odd generators is an anticommutator, all other supercommutators are commutators. The even generators generate a subalgebra which is readily recognized to be $\mathrm{o}(2m+1)\times\mathrm{sp}(2n)$.

Next we define tensor operators T^a_b by the supercommutation relations

$$\begin{aligned}[]
[G^a_b, T^c_d\}
&= \delta^c_b T^a_d - (-)^{(\eta_a+\eta_b)(\eta_c+\eta_d)}\delta^a_d T^c_b \\
&\quad - \epsilon^{\bar a}\epsilon^b(-)^{\eta_a\eta_b}\left[\delta^c_{\bar a}T^{\bar b}_d - (-)^{(\eta_a+\eta_b)(\eta_c+\eta_d)}\delta^{\bar b}_d T^c_{\bar a}\right],
\end{aligned} \tag{2.8}$$

where the supercommutator $[\ ,\ \}$ denotes

$$[G^a_b, T^c_d\} = G^a_b T^c_d - (-)^{(\eta_a+\eta_b)(\eta_c+\eta_d)} T^c_d G^a_b. \tag{2.9}$$

It then immediately follows from Eq. (2.8) that

$$\left[G^a_b, \sum_c T^c_c\right] = 0, \tag{2.10}$$

i.e., $\Sigma_c T^c_c$ is an *invariant*. Moreover, one proves just as easily that if U and V are tensors then so is UV, where

$$(UV)^a_b \equiv \sum_c U^a_c V^c_b[c], \tag{2.11}$$

and we introduce the convenient abbreviation

$$[a] \equiv (-)^{\eta_a}. \tag{2.12}$$

Clearly the generators themselves are a tensor and so is the jth power of the generators defined by

$$(G^j)^a_b = \sum_c (G^{j-1})^a_c G^c_b[c], \quad j\geqslant 1, \tag{2.13}$$

with

$$(G^0)^a_b \equiv \delta^a_b[b]. \tag{2.14}$$

Finally, therefore,

$$\sum_c (G^j)^c_c \tag{2.15}$$

are invariants and will be referred to as jth degree Casimir operators. Because the generators are antisymmetric, the linear Casimir operator vanishes and all odd-degree Casimir operators can be expressed in terms of those of even degree.

It is clear that all of the concepts described above continue to be valid if all indices are restricted to range from $-(m+n)$ to $+(m+n)$, zero *excluded*. This corresponds to the orthosymplectic superalgebra $\mathrm{osp}(2m/2n)$ with the even subalgebra being $\mathrm{o}(2m)\times\mathrm{sp}(2n)$.

Similarly, if the indices are restricted to range over positive values only, one obtains the general linear superalgebra $\mathrm{u}(m/n)$ with the even subalgebra being $\mathrm{u}(m)\times\mathrm{u}(n)$. Of course, the antisymmetry condition Eq. (2.6) no longer applies and independent odd-degree Casimir operators exist. The Kronecker symbols in the second line of Eqs. (2.1) and (2.8) now necessarily vanish, resulting in much simpler supercommutation relations.

III. THE PERELOMOV–POPOV MATRIX

The generators of the Cartan subalgebra are given in the Racah basis by G^a_a, $1\leqslant a\leqslant m+n$ (note that $G^{\bar a}_{\bar a} = -G^a_a$ in the orthosymplectic case), and state vectors in the representation space may be taken as simultaneous eigenvectors of all the G^a_a:

$$G^a_a|\mathbf{w}\rangle = w_a|\mathbf{w}\rangle, \tag{3.1}$$

$$\mathbf{w} = (w_{m+n}, w_{m+n-1},\dots,w_2, w_1), \quad w_{\bar a} = -w_a, \tag{3.2}$$

where $\mathbf{w}$ is called the weight. We consider representations for which $G^{a\dagger}_a = G^a_a$ so that the w_a are real. An ordering of the weights may be introduced. We shall call $\mathbf{w}'$ higher than $\mathbf{w}$ if the first nonvanishing component of $\mathbf{w}'-\mathbf{w}$, starting from the left, is positive. It follows from Eq. (2.8) that

$$T^c_d|\mathbf{w}\rangle = |\widetilde{\mathbf{w}}\rangle, \ \widetilde w_a - w_a = \delta^c_a - \delta^a_d + \delta^{\bar d}_a - \delta^a_{\bar c}, \tag{3.3}$$

which leads to the classification

$$T^c_d \text{ is a } \begin{Bmatrix}\text{raising}\\ \text{weight}\\ \text{lowering}\end{Bmatrix} \text{ tensor operator if } \begin{Bmatrix} c>d \\ c=d \\ c<d\end{Bmatrix}. \tag{3.4}$$

From now we consider representations possessing a unique highest-weight vector $|\mathbf{h}\rangle$, i.e.,

$$T^a_b|\mathbf{h}\rangle = \delta^a_b t_a|\mathbf{h}\rangle, \quad a\geqslant b, \tag{3.5}$$

where t_a denotes the eigenvalue of T^a_a. In particular,

$$G^a_b|\mathbf{h}\rangle = \delta^a_b h_a|\mathbf{h}\rangle, \quad a\geqslant b. \tag{3.6}$$

Consider now the tensor GT, and let f_a denote the eigenvalue of $(GT)^a_a$. We have, therefore, when applied to $|\mathbf{h}\rangle$,

$$\begin{aligned}
f_a &= \sum_{b=b_{\min}}^{a} [b]\, G^a_b T^b_a \\
&= [a]\, G^a_a T^a_a + \sum_{b=b_{\min}}^{a-1}[b]\,[G^a_b, T^b_a\} \\
&= [a]\, h_a t_a + \sum_{b=b_{\min}}^{a-1}\{[b]\, t_a - [a]\, t_b + \delta^{\bar a}_b(t_{\bar a} - t_a)\} \\
&= l_a t_a + p_a t_{\bar a} - [a]\sum_{b=b_{\min}}^{a-1} t_b,
\end{aligned} \tag{3.7}$$

where

$$p_a \equiv \sum_{b=b_{\min}}^{a-1}\delta^{\bar a}_b, \tag{3.8}$$

$$l_a \equiv [a]\, h_a - p_a + \sum_{b=b_{\min}}^{a-1}[b], \tag{3.9}$$

with $b_{\min}$ equal to 1 for the general linear, and to $-(m+n)$ for the orthosymplectic superalgebra.

Equation (3.7) may be rewritten in obvious matrix notation as

$$f = At, \tag{3.10}$$

where A is the Perelomov–Popov matrix given by

$$A_{ab} = l_a\,\delta_{ab} + p_a\,\delta_{\bar{a}b} - [a]\,\theta_{ab}, \tag{3.11}$$

with

$$\theta_{ab} = \begin{cases} 1 & \text{for } a > b, \\ 0 & \text{for } a \leqslant b. \end{cases} \tag{3.12}$$

Note that A is a triangular $N \times N$ matrix, with N the dimension of the defining representation of the relevant superalgebra, i.e., $N = m + n$ for $\mathrm{u}(m/n)$ and $N = p + 2n$ for $\mathrm{osp}(p/2n)$.

Equation (3.10) gives the eigenvalues of $(GT)^a_a$ in terms of the eigenvalues of T^b_b; by repeated iteration we obtain

$$(G^j)^a_a = \sum_b (A^j)_{ab}\,[b], \tag{3.13}$$

so that the eigenvalue of the jth degree Casimir operator is

$$C_j = \sum_{a,b} (A^j)_{ab}\,[b]. \tag{3.14}$$

The matrix A may be diagonalized as

$$(X^{-1}AX)_{ab} = l_a\,\delta_{ab}, \tag{3.15}$$

where X_{ab} is the ath component of the eigenvector of A to the eigenvalue l_b. Consequently,

$$C_j = \sum_a (l_a)^j Q_a P_a, \tag{3.16}$$

where

$$Q_a \equiv \sum_b X_{ba}, \quad P_a \equiv \sum_b (X^{-1})_{ab}\,[b]. \tag{3.17}$$

The explicit evaluation of $Q_a P_a$ is given in the following sections.

IV. THE osp($2m+1/2n$) SUPERALGEBRA

In this section, we evaluate $Q_a P_a$ in the case of the orthosymplectic superalgebra $\mathrm{osp}(2m+1/2n)$. With the indices ranging from $-(m+n)$ to $+(m+n)$, zero included, the Perelomov–Popov matrix A becomes [see Eqs. (3.8)–(3.12)]

$$A_{ab} = l_a\delta_{ab} + \theta_{a0}\delta_{\bar{a}b} - [a]\,\theta_{ab}, \tag{4.1}$$

$$l_a = [a](h_a + a + m - \theta_{a0}) + 4m\theta_{am} - n, \tag{4.2}$$

and therefore the equation defining X_{ba} is

$$(l_b - l_a)\,X_{ba} = [b]\,Q^{b-1}_a - \theta_{b0}\,X_{\bar{b}a} \tag{4.3}$$

with

$$Q^b_a \equiv \sum_{c=-m-n}^{b} X_{ca}. \tag{4.4}$$

We assume that all the eigenvalues l_a are distinct and come back to the degenerate case later. It is then clear that X_{ba} vanishes for $b < a$ while X_{aa} is arbitrary. Without loss of generality, we set $X_{aa} = 1$. For $b > a$, we must consider various possibilities.

Case I: $b > a \geqslant 0$ or $0 \geqslant b > a$ or $b > \bar{a} > 0$.

In this case, the last term in Eq. (4.3) vanishes so that we have

$$X_{ba} = \frac{[b]}{l_b - l_a}\,Q^{b-1}_a. \tag{4.5}$$

Hence

$$Q^b_a = X_{ba} + Q^{b-1}_a = \left(1 + \frac{[b]}{l_b - l_a}\right) Q^{b-1}_a \tag{4.6}$$

with the solution

$$Q^b_a = \prod_{k=a+1}^{b} \left(1 + \frac{[k]}{l_k - l_a}\right) \tag{4.7}$$

for $b > a \geqslant 0$ or $0 \geqslant b \geqslant a$, and

$$Q^b_a = Q^{\bar{a}}_a \prod_{k=a+1}^{b} \left(1 + \frac{[k]}{l_k - l_a}\right) \tag{4.8}$$

for $b > \bar{a} > 0$.

Case II: $\bar{a} \geqslant b > 0$.

In this case, the last term in Eq. (4.3) contributes so that we have

$$X_{ba} = \frac{[b]}{l_b - l_a}\,Q^{b-1}_a - \frac{1}{l_b - l_a}\,X_{\bar{b}a} \tag{4.9}$$

and

$$Q^b_a = \left(1 + \frac{[b]}{l_b - l_a}\right) Q^{b-1}_a - \frac{1}{l_b - l_a}\,X_{\bar{b}a}. \tag{4.10}$$

It should be noted that $X_{\bar{b}a}$ in these equations is known from Eqs. (4.5) and (4.7). Iteration of Eq. (4.10) yields

$$Q^b_a = \prod_{k=a+1}^{b} \left(1 + \frac{[k]}{l_k - l_a}\right) - \frac{1}{l_b - l_a}\,X_{\bar{b}a} - \sum_{c=1}^{b-1} X_{\bar{c}a}\,\frac{1}{l_c - l_a} \prod_{k=c+1}^{b} \left(1 + \frac{[k]}{l_k - l_a}\right), \tag{4.11}$$

and the sum may be evaluated in closed form. In particular, for $b = \bar{a}$ we get

$$Q^{\bar{a}}_a = \left(1 + \frac{[a]+1}{l_{\bar{a}} - l_a}\right) \prod_{\substack{k=a+1 \\ \neq 0}}^{\bar{a}-1} \left(1 + \frac{[k]}{l_k - l_a}\right). \tag{4.12}$$

Collecting all these results, we conclude

$$Q_a \equiv Q^{m+n}_a = \left\{1 + \theta_{\bar{a}0}\,\frac{[a]+1}{l_{\bar{a}} - l_a}\right\} \times \prod_{\substack{k=a+1 \\ \neq 0,\bar{a}}}^{m+n} \left(1 + \frac{[k]}{l_k - l_a}\right). \tag{4.13}$$

A very similar calculation leads to

$$P_a = [a]\left\{1 + \theta_{a0}\,\frac{[a]+1}{l_{\bar{a}} - l_a}\right\} \times \prod_{\substack{k=\bar{m}+\bar{n} \\ \neq 0,\bar{a}}}^{a-1} \left(1 + \frac{[k]}{l_k - l_a}\right), \tag{4.14}$$

and therefore

$$Q_a P_a = [a]\left\{1 + (1 - \delta_{a0})\,\frac{[a]+1}{l_{\bar{a}} - l_a}\right\} \times \prod_{k \neq 0,\bar{a},a} \left(1 + \frac{[k]}{l_k - l_a}\right). \tag{4.15}$$

V. THE osp(2m/2n) SUPERALGEBRA

In this section, we evaluate $Q_a P_a$ in the case of the orthosymplectic superalgebra osp($2m/2n$). With the indices ranging from $-(m+n)$ to $+(m+n)$, zero excluded, the Perelomov–Popov matrix A has the same form as in the previous section except that l_a is now given by [see Eqs. (3.8) and (3.9)]

$$l_a = [a](h_a + a + m - \theta_{a0}) + 4m\theta_{am} - n - \theta_{a0}. \quad (5.1)$$

If one now follows precisely the same steps as in the previous section (keeping in mind that zero is excluded from the range of indices), one obtains

$$Q_a P_a = [a] \left\{ 1 + \frac{[a]-1}{l_{\bar{a}} - l_a} \right\} \prod_{k \neq \bar{a},a} \left(1 + \frac{[k]}{l_k - l_a} \right). \quad (5.2)$$

VI. THE u(m/n) SUPERALGEBRA

In this section, we evaluate $Q_a P_a$ in the case of the general linear superalgebra u(m/n). With the indices ranging from 1 to $m+n$, the Perelomov–Popov matrix A becomes [see (3.8)–(3.12)]

$$A_{ab} = l_a \delta_{ab} - [a]\, \theta_{ab}, \quad (6.1)$$

$$l_a = [a](h_a + a - 1 - 2m\theta_{am}). \quad (6.2)$$

The calculation described in Sec. IV now simplifies drastically, and one finds

$$Q_a P_a = [a] \prod_{k \neq a} \left(1 + \frac{[k]}{l_k - l_a} \right). \quad (6.3)$$

VII. CONCLUSION

Inserting the expression for $Q_a P_a$ from Eq. (4.15), (5.2) and (6.3), respectively, into Eq. (3.16) yields the final answers for the eigenvalue of the jth degree Casimir operator for the various superalgebras as quoted in the Introduction. We make the following comments.

It would appear that these results can only be used in the absence of degeneracy (recall that it was assumed in the diagonalizing of the matrix A that its eigenvalues were all distinct). However, we know from the definition of the C_j by Eq. (2.15) that they must in fact be a polynomial in the components of the weight. Hence all the denominators must, in fact, divide out and, in this sense, the results are valid in the degenerate case as well.

The general linear algebra u(m) may be thought of as a special case of the u(m/n) superalgebra for $n = 0$. Similarly the orthogonal algebras o($2m$) and o($2m+1$) are special cases of the orthosymplectic superalgebras o($2m/2n$) and o($2m+1/2n$) for $n = 0$, while the symplectic algebra sp($2n$) is a special case of the o($2m/2n$) superalgebra for $m = 0$. Our results for C_j reduce to the corresponding results for the ordinary algebras when m or n is set equal to zero. In making the comparison with existing formulas in the literature for the ordinary algebras, some care is needed with respect to the conventions on ordering of weights. Thus our results are in direct agreement with Nwachuku and Rashid,[4] who use the same ordering convention, and are in agreement with Okubo[3] after the difference in the ordering conventions is taken into account.

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The use of comparison filters in linear filter theory

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In the present paper, it is shown how the linear filter equation for a given correlation coefficient can be solved in terms of the solution of the filter equation with a different correlation coefficient. The second filter is called a comparison filter. One obtains an integral equation for the difference of the two filters in terms of the difference of the two correlation functions and the solution of the comparison filter. Thus if the comparison filter is known and its correlation coefficient is close to that of the desired filter, one may regard the comparison filter as being an approximation to it. The difference of the two filters is then small and perturbation expansions or variational principles for the difference may be expected to give better results than if one did not use a comparison filter. The difference in the solutions of the two filter equations may also be regarded as the change (or error) in the filter due to a change (or error) in the correlation coefficient. Our result is obtained by pressing the close analogy of the filter equation to the Gel'fand–Levitan equation of inverse spectral theory. Another result of the use of comparison filters is to show that the filter equation for the difference of filters satisfies a possibly useful grouplike property.

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I. INTRODUCTION

In Ref. 1, Kay and Moses treated the Gel'fand–Levitan equation of the inverse spectral theory problem from a very general point of view and observed that the Gel'fand–Levitan equation was a generalization of the filter equation of that time, namely, the Wiener–Hopf equation. This observation continues to hold for more general filters, for example, the Kalman filter. Recently, one of us (Moses, Ref. 2) gave a general scheme for introducing comparison potentials for which the solution of the corresponding Gel'fand–Levitan equation is known. The solution of any other Gel'fand–Levitan equation could be expressed in terms of the known solution through the use of an integral equation for the difference of the known and sought for Gel'fand–Levitan kernels. The use of comparison potentials led to perturbation schemes and variational principles which, in principle at least, led to more accurate approximations for the desired Gel'fand–Levitan kernel.

The purpose of the present paper is to give the analog for the filter equation. It is shown how the linear filter equation for a given correlation coefficient can be solved in terms of the solution of the filter equation with a different correlation coefficient. The second filter is called a comparison filter. One obtains an integral equation for the difference of the two filters in terms of the difference of the two correlation functions and the solution of the comparison filter. Thus if the comparison filter is known and its correlation coefficient is close to that of the desired filter, one may regard the comparison filter as being an approximation to it. The difference of the two filters is then small and perturbation expansions or variational principles for the difference may be expected to give better results than if one did not use a comparison filter.

The difference may also be regarded as the change (or error) in the filter due to a change (or error) in the correlation coefficient. Another result of the use of a comparison filter is to show that the filter equation for the difference of filters satisfies a possibly useful grouplike property.

II. THE FILTER EQUATION AS A GEL'FAND–LEVITAN EQUATION

In dealing with the filter equation, we shall use standard notation as given, for example, in Kailath's monograph (Ref. 3). The filter equation is then

$$h(t,s) = K(t,s) - \int_{t_0}^{t} h(t,\tau) K(\tau,s)\, d\tau \qquad (t_0 \leqslant s \leqslant t \leqslant t_f). \tag{1}$$

In Eq. (1), $h(t,s)$ is the filter matrix $h(t,s) = \{h_{ij}(t,s)\}$, and the matrix $K(t,s) = \{K_{ij}(t,s)\}$ is related to the signal correlation matrix $R_y(t,s)$ by

$$R_y(t,s) = I_p \delta(t-s) + K(t,s) \equiv E y(t) y'(t). \tag{2}$$

The Gel'fand–Levitan equation, as treated in Ref. 1, is identical to the filter equation in which $h(t,s)$ is the negative of the Gel'fand–Levitan kernel $\langle t | K | s \rangle$, and the matrix $K(t,s)$ is the driving kernel $\langle t | \Omega | s \rangle$ of Ref. 1. To press the analogy even further, it is useful to define the filter matrix as having the triangularity property

$$h(t,s) = 0 \quad \text{for} \quad s > t. \tag{3}$$

In the space of observables which include the signals $y(t)$, let us define the operators in terms of integral operators with kernels. For example, if $f(t)$ is in the space, we shall write

$$h f(t) \quad \int_{t_0}^{t} h(t,s) f(s)\, ds, \qquad R_y f(t) = \int_{t_0}^{t_f} R_y(t,s) f(s)\, ds, \tag{4}$$

and so on. Let us define the operator U by

$$U f(t) = f(t) - h f(t). \tag{5}$$

In particular, if $y(t)$ is a signal,

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$$Uy(t) = y(t) - \hat{z}(t), \tag{6}$$

where $\hat{z}(t) = hy(t)$ is the filtered signal. Thus $Uy(t)$ is the difference between the original noisy signal and the filtered signal.

Now let us define the operator h_0 through its kernel by

$$h_0(t,s) \equiv 0 \text{ for } s > t,$$

$$h_0(t,s) = h^{\dagger}(t,s) - K(t,s) + \int_{t_0}^{s} K(t,\tau) h^{\dagger}(\tau,s) d\tau \text{ for } t \geqslant s, \tag{7}$$

where $W^{\dagger}$ is the full adjoint of the operator W with the kernel $W^{\dagger}(t,s)$. This full adjoint, as opposed to the matrix adjoint W', is defined with respect to the full inner product

$$(g,f) = \int_{t_0}^{t_f} g'(t) f(t) dt, \tag{8}$$

so that $W^{\dagger}$ is defined by

$$(g, Wf) = (W^{\dagger} g, f). \tag{9}$$

Hence in terms of matrix elements,

$$W^{\dagger}_{ij}(t,s) = W^{*}_{ji}(s,t) = W'_{ij}(s,t). \tag{9a}$$

Let us define the operator U_0 by

$$U_0 f(t) = f(t) - h_0 f(t). \tag{10}$$

Then, on using Eq. (7) in the form

$$h_0 = h^{\dagger} - K - Kh^{\dagger},$$

it is readily seen that the filter equation (1) is identical to

$$UR_y = U_0^{\dagger}. \tag{11}$$

In fact, this is just Eq. (1.1) of Ref. 1. In deriving Eq. (11), we have used the fact that $R_y^{\dagger} = R_y$.

One of the more surprising results of Ref. 1 is the following.

Theorem:

$$U_0 = U^{-1}. \tag{12}$$

Since the proof is given in Ref. 1, we shall not repeat it here. Thus the filter equation, together with the triangularity conditions on h and h_0, is equivalent to

$$UR_y U^{\dagger} = I \tag{13}$$

together with the triangularity conditions. In Eq. (13) I is, of course, the identity operator.

Eq. (13), which in the context of Ref. 1 is the Gel'fand–Levitan equation in its most general form, is the basis of the further work in the present paper. From Eq. (2) and (6), it is seen that Eq. (13) leads to

$$E\{[y(t) - \hat{z}(t)][y'(s) - \hat{z}'(s)]\} = I_p \delta(t-s), \tag{14}$$

which is the analog of the completeness relation obtained from the Gel'fand–Levitan equation.

III. THE BASIC FORMULAS INVOLVING THE USE OF THE COMPARISON FILTER

Let us now consider the entire set of correlation functions $\{R_y = I + K\}$. Consider any two of them which we shall call $R_y^{(n)} = I + K^{(n)}$ and $R_y^{(m)} = I + K^{(m)}$, respectively. (Though we have labeled the correlation functions as though they had come from a discrete set, the set is not denumerable and a continuous label could have been used.)

Let us define $U^{(n)}, U_0^{(n)} = [U^{(n)}]^{-1}$ as being the filter operators associated with $R_y^{(n)}$, and define similar quantities for the superscript m.

Furthermore, define

$$U^{(n,m)} = U^{(n)} U_0^{(m)} = I - h^{(n,m)},$$

$$U_0^{(n,m)} = [U^{(n,m)}]^{-1} = U^{(m)} U_0^{(n)}$$

$$= U^{(m,n)} = I - h^{(m,n)}. \tag{15}$$

It should be noted that because of the triangularity properties of $h^{(n)}$ and $h_0^{(n)}$ and the fact that

$$h^{(n,m)} = h^{(n)} + h_0^{(m)} - h^{(n)} h_0^{(m)}, \tag{16}$$

which follows from Eq. (15), it follows that the kernel of the operator $h^{(n,m)}$ also satisfies the triangularity property

$$h^{(n,m)}(t,s) = 0 \qquad \text{for } s > t. \tag{17}$$

From Eq. (13) and (15),

$$U^{(n,m)} U^{(m)} R_y^{(n)} U^{(m)\dagger} U^{(n,m)\dagger} = I. \tag{18}$$

But

$$R_y^{(n)} = R_y^{(n)} - R_y^{(m)} + R_y^{(m)}. \tag{19}$$

Furthermore,

$$U^{(m)} R_y^{(m)} U^{(m)\dagger} = I. \tag{20}$$

Thus

$$U^{(n,m)} R_y^{(n,m)} U^{(n,m)\dagger} = I, \tag{21}$$

where

$$R_y^{n,m} = I + U^{(m)} [R_y^{(n)} - R_y^{(m)}] U^{(m)\dagger}. \tag{22}$$

Equation (21) is precisely of the form Eq. (13). Thus, finally,

$$h^{(n,m)}(t,s) = K^{(n,m)}(t,s) - \int_{t_0}^{t} h^{(n,m)}(t,\tau) K^{(n,m)}(\tau,s) d\tau. \tag{23}$$

In Eq. (23), $K^{(n,m)}(t,s)$ is the kernel of the operator $K^{(n,m)}$ given by

$$K^{(n,m)} = U^{(m)} [R_y^{(n)} - R_y^{(m)}] U^{n\dagger}$$

$$= U^{(m)} [K^{(n)} - K^{(m)}] U^{(m)\dagger}. \tag{24}$$

Equation (23) is the principal result of the paper. It is an equation of the type used for filters and depends upon the difference between two correlations and knowledge of a filter associated with one of them. We may regard the filter labeled by n as being the one we wish to approximate by a known filter labeled by m. If the correlations of filter n and m are close, one expects the operator $h^{(n,m)}$ to be small in some suitable sense. Perturbation theory or some other approximation based on the assumption that the correlations are close and thus $h^{(n,m)}$ is small may then be expected to work better than solving the filter equation directly for n. Having obtained $h^{(n,m)}$, one obtains $U^{(n,m)} = I - h^{(n,m)}$ and finally $U^{(n)} = U^{(n,m)} U^{(m)}$. Since $h^{(n,m)}$ satisfies the filter equation with a kernel such that $I + K^{(n,m)}$ is positive definite, one can obtain a variational principle for the solution. This variational principle is discussed in Ref. 4. Though we shall not repeat it here, a quantity which plays an important role is $\operatorname{tr} h^{(n)}(t,t)$. In Ref. 4, it is shown that

$$\mathrm{tr}\, h^{(n)}(t,t) = \mathrm{tr}\, E\,[z(t) - \hat{z}^{(n)}(t)][z(t) - \hat{z}^{(n)}(t)]' + \mathrm{tr}\, H(t)G(t)C(t). \tag{25}$$

In Eq. (25), we have used the notation for the Kalman filter as given, for example, in Ref. 3. Using the above techniques, one can show

$$\mathrm{tr}\, h^{(n,m)}(t,t) = \mathrm{tr}\, h^{(n)}(t,t) - \mathrm{tr}\, h^{(m)}(t,t). \tag{26}$$

Hence one can calculate $\mathrm{tr}\, h^{(n)}(t,t)$ from a knowledge of the mth filter and from the solution of Eq. (23).

IV. THE GROUPLIKE PROPERTY OF THE FILTER. THE NOTION OF "PATHS" IN THE SET OF FILTERS

As we have seen in the preceding discussion, the operator $U^{(n,m)}$ allows us to go from the mth filter to the nth filter by means of a filter equation for $h^{(n,m)}$ in terms of the difference in the correlation functions of the nth and mth filter and the solution of the filter equation for the mth filter. This result is independent of the closeness of the correlation functions of the mth filter to that of the nth filter.

From Eq. (15), one can go from the mth filter to the nth filter through an arbitrary set of intermediate filters, since

$$U^{(n,m)} = U^{(n,n_1)}U^{(n_1,n_2)}U^{(n_2,n_3)}\ldots U^{(n_p,m)}, \tag{27}$$

where p is the number of intermediate filters. The correlations for the intermediate filters are arbitrary. Each set of intermediate filters will be said to constitute a "path" from the mth filter to the nth filter. Since the set of intermediate filters is arbitrary, the method of constructing the nth filter from the mth filter through the use of intermediate filters is "path independent."

The relation (27) is very similar to the composition rule for the conditional probabilities of a Markov chain. It may be possible to get another formulation for filter theory from these notions. For example, one might consider the case where the intermediate filters differ from each other by an amount which is very small. One might then be able to go to the limit of an infinite number of intermediate filters which differ from each other by a decreasing amount.

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New representations for the spherical tensor gradient and the spherical delta function

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In this article, we analyze representations for the product $\mathcal{Y}_{l_1}^{m_1}(\nabla) F_{l_2}^{m_2}(\mathbf{r})$ with $\mathcal{Y}_l^m(\nabla)$ specifying a solid harmonic whose argument is the nabla operator $\partial/\partial\mathbf{r}$ instead of the vector $\mathbf{r}$. Since both $\mathcal{Y}_{l_1}^{m_1}(\nabla)$ and $F_{l_2}^{m_2}(\mathbf{r})$ are irreducible spherical tensors, we can use angular momentum algebra for evaluating the product. Accordingly, the problem of finding a representation for the product is reduced to the determination of the radial functions generated by the product. Analytical expressions for these radial functions are derived by direct differentiation and with the help of Fourier transforms. Closely related to the spherical tensor gradient $\mathcal{Y}_l^m(\nabla)$ is the spherical delta function $\delta_l^m(\mathbf{r})$. We derive new representations for δ_l^m by considering convolution integrals involving B functions. These functions are closely related to the modified Bessel functions and also to the Yukawa potential $e^{-\alpha r}/r$. We show that the definition of the B functions can be extended to include a large class of derivatives of the delta functions, where the spherical delta function is just a special case.

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I. INTRODUCTION

If one analyzes polynomials in the Cartesian components x, y, and z of a vector $\mathbf{r}$, one can classify certain subsets of them in terms of some transformation properties or symmetries. For instance, one may consider the class of homogeneous polynomials of degree l, i.e., those polynomials which satisfy

$$P_l(\eta x,\eta y,\eta z) = \eta^l P_l(x,y,z) . \tag{1.1}$$

A special subset of these homogeneous polynomials of degree l are the so-called harmonic polynomials $H_l(x,y,z)$ which satisfy Laplace's equation

$$\nabla^2 H_l(x,y,z) = \left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right\} H_l(x,y,z) = 0 . \tag{1.2}$$

For a given value of l, only $2l+1$ linearly independent harmonic polynomials exist.[1] Hence it is possible to span the space of harmonic polynomials by the so-called regular solid harmonics

$$\mathcal{Y}_l^m(\mathbf{r}) = r^l\, \mathcal{Y}_l^m(\theta,\phi) , \tag{1.3}$$

where $Y_l^m(\theta,\phi)$ is a spherical harmonic, i.e., by polynomials in x, y, and z that transform under rotations like irreducible spherical tensors.

Obviously, the same classification scheme can be applied if we do not consider polynomials in x, y, and z but instead polynomials in the Cartesian components $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$ of the gradient ∇. In this article, we want to analyze properties of a differential operator, the spherical tensor gradient $\mathcal{Y}_l^m(\nabla)$, which transforms under rotations like a spherical tensor of rank l.[2] This differential operator is obtained from the regular solid harmonic $\mathcal{Y}_l^m(\mathbf{r})$ by replacing x, y, and z by $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$.

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This spherical tensor gradient was, in principle, already used by Hobson in his book on spherical harmonics.[3] Later it was studied by Santos,[4] Rowe,[5] and Bayman[6] in connection with the derivation of addition theorems and multiple expansions, and by Stuart,[7] who investigated the connection between nonclassical integrals of Bessel functions and delta functions. Fieck[8] used the spherical tensor gradient to define a special class of Gaussian-type atomic orbitals, and recently we could show that some multicenter integrals over nonscalar exponential-type functions can be generated from the corresponding integrals over scalar functions by applying the spherical tensor gradient.[9]

In this article, we want to derive compact analytical representations for the expression

$$\mathcal{Y}_{l_1}^{m_1}(\nabla) F_{l_2}^{m_2}(\mathbf{r}) , \tag{1.4}$$

where the function $F_{l_2}^{m_2}(\mathbf{r})$ is also an irreducible tensor. Although such expressions as (1.4) have been investigated previously,[4,6,7] we shall show that the hitherto known results can still be improved.

Closely related to the spherical tensor gradient is the so-called spherical delta function

$$\delta_l^m(\mathbf{r}) = \frac{(-1)^l}{(2l-1)!!}\, \mathcal{Y}_l^m(\nabla)\delta(\mathbf{r}) , \tag{1.5}$$

where the differentiation is to be understood in the sense of generalized functions.[10] We want to derive some new representations for the spherical delta function which can be considered to be a generalization of the well-known fact that the Yukawa potential $e^{-\alpha r}/r$ is the Green's function of the modified Helmholtz equation. In our approach, we exploit the fact that convolution integrals involving the Yukawa potential may be considered to be special cases of a more general class of convolution integrals involving the so-called B functions.[11,12] B functions are exponential-type functions that are closely related to the modified Bessel function of the

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second kind. B functions were investigated in connection with multicenter problems.[9,11–14] It was found that multicenter integrals of B functions are less complicated than those of other exponential-type functions as, for instance, Slater-type functions. Recently we could show that the advantageous properties of B functions in multicenter problems can be explained in terms of their extremely simple Fourier transform.[9] The Fourier transform of B functions will also be of considerable importance in this article. The fact that the spherical delta function δ_l^m can be expressed in terms of B functions is, as we shall show later, a direct consequence of the analytical structure of the Fourier transform.

II. DEFINITIONS AND BASIC PROPERTIES

For the commonly occurring special functions of mathematical physics we shall use the notations and conventions of Magnus, Oberhettinger, and Soni,[15] unless explicitly stated.

The spherical harmonics $Y_l^m(\theta,\phi)$ are defined using the phase convention of Condon and Shortley,[16] i.e., they are given by the expression

$$Y_l^m(\theta,\phi) = i^{m+|m|}\left[\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta)\, e^{im\phi}. \tag{2.1}$$

Here, $P_l^{|m|}(\cos\theta)$ is an associated Legendre polynomial.

$$P_l^m(x) = (1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}\frac{(x^2-1)^l}{2^l l!} = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x). \tag{2.2}$$

For the irregular solid harmonic, we write

$$\mathscr{Z}_l^m(\mathbf{r}) = r^{-l-1}\, Y_l^m(\theta,\phi). \tag{2.3}$$

The regular solid harmonic $\mathscr{Y}_l^m(\mathbf{r})$ was already defined in Eq. (1.3).

For the integral over the product of three spherical harmonics, the so-called Gaunt coefficient, we write

$$\langle l_3 m_3|l_2 m_2|l_1 m_1\rangle = \int Y_{l_3}^{m_3 *}(\Omega)\, Y_{l_2}^{m_2}(\Omega)\, Y_{l_1}^{m_1}(\Omega)\, d\Omega. \tag{2.4}$$

These Gaunt coefficients may be expressed in terms of Clebsch–Gordan coefficients[17] or $3jm$-symbols

$$\langle lm|l_1m_1|l_2m_2\rangle = \left[\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}\right]^{1/2} C_{0\,0\,0}^{l_1 l_2 l}\, C_{m_1 m_2 m}^{l_1 l_2 l} \tag{2.5}$$

$$= (-1)^m\left[\frac{(2l_1+1)(2l_2+1)(2l+1)}{4\pi}\right]^{1/2}\begin{pmatrix} l_1 & l_2 & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_1 & l_2 & l\\ m_1 & m_2 & -m\end{pmatrix}. \tag{2.6}$$

With the help of these Gaunt coefficients, we can linearize the product of two spherical harmonics:

$$Y_{l_1}^{m_1}(\theta,\phi)\, Y_{l_2}^{m_2}(\theta,\phi) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle lm_1+m_2|l_1m_1|l_2m_2\rangle\, Y_l^{m_1+m_2}(\theta,\phi). \tag{2.7}$$

The symbol $\Sigma^{(2)}$ indicates that the summation is to be performed in steps of two. The summation limits in Eq. (2.7) are given by[18]

$$l_{\max} = l_1 + l_2, \tag{2.8a}$$

$$l_{\min} = \begin{cases} \max(|l_1-l_2|,|m_1+m_2|) \\ \text{if } l_{\max} + \max(|l_1-l_2|,|m_1+m_2|) \text{ is even, and} \\ \max(|l_1-l_2|,|m_1+m_2|)+1 \\ \text{if } l_{\max} + \max(|l_1-l_2|,|m_1+m_2|) \text{ is odd.} \end{cases} \tag{2.8b}$$

In the sequel, we shall frequently use the following combinations of the three angular momentum quantum numbers l_1, l_2, and l:

$$\Delta l = (l_1+l_2-l)/2, \tag{2.9a}$$

$$\Delta l_1 = (l-l_1+l_2)/2, \tag{2.9b}$$

$$\Delta l_2 = (l+l_1-l_2)/2, \tag{2.9c}$$

$$\sigma(l) = (l_1+l_2+l)/2. \tag{2.9d}$$

It is an immediate consequence of the summation limits in Eq. (2.7) that these quantities are always positive integers or zero.

In this article, we want to use the symmetric version of the Fourier transformation, i.e., a given function $f(\mathbf{r})$ and its Fourier transform $\bar f(\mathbf{p})$ are connected by the relationships

$$\bar f(\mathbf{p}) = (2\pi)^{-3/2}\int e^{-i\mathbf{p}\cdot\mathbf{r}} f(\mathbf{r})\, d^3\mathbf{r}, \tag{2.10}$$

$$f(\mathbf{r}) = (2\pi)^{-3/2}\int e^{i\mathbf{r}\cdot\mathbf{p}}\bar f(\mathbf{p})\, d^3\mathbf{p}. \tag{2.11}$$

For the explicit evaluation of such Fourier integrals we use the Rayleigh expansion of a plane wave in terms of spherical Bessel functions and spherical harmonics:

$$e^{\pm i\mathbf{x}\cdot\mathbf{y}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(\pm i)^l j_l(xy)\, Y_l^{m*}(\mathbf{x}/x) Y_l^m(\mathbf{y}/y). \tag{2.12}$$

The spherical Bessel function is related to a Bessel function of the first kind by

$$j_n(z) = (\pi/2z)^{1/2} J_{n+1/2}(z). \tag{2.13}$$

If $K_\nu(z)$ stands for the modified Bessel function of the second kind, we define the reduced Bessel function with arbitrary order ν by

$$\hat{k}_\nu(z) = (2/\pi)^{1/2} z^\nu K_\nu(z) . \tag{2.14}$$

In the case of half-integral orders, $\nu = n - \frac{1}{2}$, $n\in\mathbb{N}$, the reduced Bessel function can be represented by an exponential multiplied by a polynomial[19]:

$$\hat{k}_{n-1/2}(z) = e^{-z} \sum_{q=1}^{n} \frac{(2n-q-1)!}{(q-1)!(2n-2q)!} z^{q-1} . \tag{2.15}$$

As we found out recently, the polynomial part in Eq. (2.15) has also been investigated independently in the mathematical literature.[20] There, the notation

$$\theta_n(z) = e^z \hat{k}_{n+1/2}(z) \tag{2.16}$$

is used. Together with some other closely related polynomials, the polynomials $\theta_n(z)$ are called Bessel polynomials. They find applications in such diverse fields as number theory, statistics and the analysis of complex electrical networks.[20]

As a nonscalar generalization of the reduced Bessel function, the so-called B function was introduced[21]:

$$B_{n,l}^m(\alpha,\mathbf{r}) = [2^{n+l}(n+l)!]\ \hat{k}_{n-1/2}(\alpha r)\ \mathcal{Y}_l^m(\alpha\mathbf{r}) . \tag{2.17}$$

In the sequel, it will be tacitly assumed that the order n of a B function will always be a positive or negative integer. The factorial in Eq. (2.17) requires that $n + l \geqslant 0$ holds. However, as we shall show later, Eq. (2.17) remains meaningful even if $n + l < 0$ holds. It is, of course, clear that such objects are no ordinary functions, but, instead, they have to be interpreted as distributions.

In this article, we shall discuss only those properties of B functions that are relevant for the representation of the spherical delta function δ_l^m, defined in Eq. (1.5), in terms of B functions. More complete treatments of the mathematical properties of B functions were given elsewhere.[9,11,12,22,23]

III. APPLICATION OF THE SPHERICAL TENSOR GRADIENT—DIRECT DIFFERENTIATION

We want to apply the spherical tensor gradient $\mathcal{Y}_l^m(\nabla)$ to a relatively large class of functions $f:\mathbb{R}^3\to\mathbb{C}$. We only require that these functions can be differentiated sufficiently often with respect to x, y, and z and that they are irreducible spherical tensors of a given rank, i.e., that these functions can be written as

$$F_l^m(\mathbf{r}) = f_l(r)\ Y_l^m(\mathbf{r}/r) . \tag{3.1}$$

In this and the next section we want to derive and analyze analytical representations for the product

$$\mathcal{Y}_{l_1}^{m_1}(\nabla)\, F_{l_2}^{m_2}(\mathbf{r}) , \tag{3.2}$$

which is just a special case of the well-studied problem of the coupling of two irreducible spherical tensors. Accordingly, we shall use angular momentum algebra in order to determine the general structure of the desired result.

Let $S_{k_1}^{\mu_1}$ and $T_{k_2}^{\mu_2}$ be the components of two sets of irreducible spherical tensor operators $S^{(k_1)}$ and $T^{(k_2)}$. Then the tensor product of $S^{(k_1)}$ and $T^{(k_2)}$ is defined by the sum[24]

$$[S^{(k_1)}\times T^{(k_2)}]_k^\mu = \sum_{\mu_1\mu_2} C_{\mu_1\mu_2\mu}^{k_1k_2k}\ S_{k_1}^{\mu_1}\ T_{k_2}^{\mu_2} . \tag{3.3}$$

With the help of the orthogonality properties of the Clebsch–Gordan coefficients, this relationship can be inverted to yield

$$S_{k_1}^{\mu_1}\ T_{k_2}^{\mu_2} = \sum_k C_{\mu_1\mu_2\mu_1+\mu_2}^{k_1k_2k}\ [S^{(k_1)}\times T^{(k_2)}]_k^{\mu_1+\mu_2} . \tag{3.4}$$

The summation limits in Eq. (3.4) are determined by the selection rules satisfied by the Clebsch–Gordan coefficients. Comparison of Eqs. (3.2) and (3.4) shows that we have to expect a result of the following general structure:

$$\mathcal{Y}_{l_1}^{m_1}(\nabla)F_{l_2}^{m_2}(\mathbf{r}) = \sum_l C_{m_1m_2m_1+m_2}^{l_1l_2l}\ [\mathcal{Y}^{(l_1)}(\nabla)\times F^{(l_2)}(\mathbf{r})]_l^{m_1+m_2} . \tag{3.5}$$

The spherical harmonics $Y_l^m(\theta,\phi)$ are a complete orthonormal set in the Hilbert space of functions that are square integrable with respect to an integration over the surface of the unit sphere in $\mathbb{R}^3$. Hence we can express the components of the tensor product in Eq. (3.5) in terms of a spherical harmonic multiplied by a function that depends only on the distance r:

$$[\mathcal{Y}^{(l_1)}(\nabla)\times F^{(l_2)}(\mathbf{r})]_l^{m_1+m_2} = g_{l_1l_2}^l(r) Y_l^{m_1m_2}(\mathbf{r}/r) . \tag{3.6}$$

We now exploit the fact that, under a reflection where $\mathbf{r}\to -\mathbf{r}$ and $\nabla\to -\nabla$, both sides of Eq. (3.5) must transform identically. From the fact that a spherical harmonic Y_l^m has the parity $(-1)^l$, we may conclude that $l_1 + l_2 + l$ has to be an even integer or zero or, equivalently, that the l-summation in Eq. (3.5) proceeds in steps of two. Hence we finally obtain the following structure for our desired result:

$$\mathcal{Y}_{l_1}^{m_1}(\nabla)\, F_{l_2}^{m_2}(\mathbf{r}) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\ C_{m_1m_2m_1+m_2}^{l_1l_2l}\ g_{l_1l_2}^l(r)\ Y_l^{m_1+m_2}(\mathbf{r}/r) . \tag{3.7}$$

The summation limits $l_{\min}$ and $l_{\max}$ agree with those that occur in the linearization of the product of two spherical harmonics, Eq. (2.7), and are given by Eq. (2.8).

Equation (3.7) was the starting point of the analysis of Bayman[6] who derived an explicit expression for the functions $g_{l_1l_2}^l(r)$. However, as will become clear later, it is advantageous to proceed in a different way. We define instead

$$g_{l_1l_2}^l(r) = \left[\frac{(2l_1+1)(2l_2+1)}{4\pi}\right]^{1/2} C_{000}^{l_1l_2l}\ \gamma_{l_1l_2}^l(r) . \tag{3.8}$$

The Clebsch–Gordan coefficients can now be replaced by a Gaunt coefficient, and Eq. (3.7) can be rewritten as

$$\mathcal{Y}_{l_1}^{m_1}(\nabla)\, F_{l_2}^{m_2}(\mathbf{r}) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\ \langle lm_1+m_2|l_1m_1|l_2m_2\rangle\ \gamma_{l_1l_2}^l(r) Y_l^{m_1+m_2}(\mathbf{r}/r) . \tag{3.9}$$

With the help of angular momentum algebra, the problem of deriving an explicit expression for the product (3.2) could be reduced to the determination of the functions $\gamma_{l_1l_2}^l(r)$.

Let us first consider the case that $F_l^m(\mathbf{r})$ is a tensor of rank 0, i.e., a scalar function. Then we can obtain the desired result most easily with the help of a theorem of Hobson[25]:

Let $f_n(x,y,z)$ be a homogeneous function of degree n in the variables x,y, and z, and let F be any function that depends only on $r^2 = x^2 + y^2 + z^2$. Then the application of the homogeneous differential operator $f_n(\partial/\partial x,\partial/\partial y,\partial/\partial z)$ on $F(r^2)$ can be expressed in closed form by

$$f_n\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}\right)F(r^2)$$

$$= \sum_{q=0}^{n} \frac{2^{n-2q}}{q!}\left[\left(\frac{d}{dr^2}\right)^{n-q} F(r^2)\right] \nabla^{2q} f_n(x,y,z). \quad (3.10)$$

A substantial simplification is obtained if $f_n(x,y,z)$ is a solution of Laplace's equation, because in this case only the term with $q = 0$ is different from zero. Hence if f_n stands for a solid harmonic $\mathscr{Y}_l^m$, we obtain

$$\mathscr{Y}_l^m(\nabla)F(r^2) = \left[2^l\left(\frac{d}{dr^2}\right)^l F(r^2)\right]\mathscr{Y}_l^m(r). \quad (3.11)$$

If we now set $F(r^2) = \phi(r)$, we obtain

$$\mathscr{Y}_l^m(\nabla)\phi(r) = \left[\left(\frac{1}{r}\frac{d}{dr}\right)^l \phi(r)\right]\mathscr{Y}_l^m(\mathbf{r}), \quad (3.12)$$

where we used

$$\frac{d}{dr^2} = \frac{1}{2r}\frac{d}{dr}. \quad (3.13)$$

Hobson[3] used Eqs. (3.10) and (3.11) to derive the following well-known result:

$$\mathscr{Y}_l^m(\nabla)\frac{1}{r} = (-1)^l(2l-1)!!\,\mathscr{Z}_l^m(\mathbf{r}). \quad (3.14)$$

For the treatment of the general case when the spherical tensor gradient $\mathscr{Y}_{l_1}^{m_1}(\nabla)$ is applied to an irreducible spherical tensor $F_{l_2}^{m_2}(\mathbf{r})$ or rank $l_2 > 0$, it is important to note that the functions $\gamma_{l_1 l_2}^{l}(r)$ in Eq. (3.9) do not depend upon the magnetic quantum numbers m_1 and m_2 and can be considered to be a kind of reduced matrix element in the sense of the Wigner–Eckhart theorem. Hence one can try to find an explicit representation for $\gamma_{l_1 l_2}^{l}$ for some special values of m_1 and m_2, which, because of the general structure of Eq. (3.9), then holds for all admissible values of m_1 and m_2.

The solid harmonics with $m = \pm l$ have a particularly simple structure:

$$\mathscr{Y}_l^{\pm l}(r) = \frac{i^{l\pm l}}{2^l l!}\left[\frac{(2l+1)!}{4\pi}\right]^{1/2}(x \pm iy)^l. \quad (3.15)$$

Following Bayman[6] we apply the differential operator $\mathscr{Y}_{l_1}^{l_1}(\nabla)$ to the function $F_{l_2}^{-l_2}(\mathbf{r})$. From the general rules of angular momentum coupling, it follows that for $m_1 = l_1$ and $m_2 = -l_2$ we have, in Eq. (3.9), the summation limit $l_{\min} = |l_1 - l_2|$, i.e., all possible values of l will be covered by the result. We then obtain

$$\mathscr{Y}_{l_1}^{l_1}(\nabla)F_{l_2}^{-l_2}(\mathbf{r})$$
$$= (-1)^{l_1}\frac{[(2l_1+1)!(2l_2+1)!]^{1/2}}{4\pi\,2^{l_1+l_2}\,l_1!l_2!}$$
$$\times\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^{l_1}\frac{f_{l_2}(r)}{r^{l_2}}(x-iy)^{l_2}. \quad (3.16)$$

In order to perform the differentiation, we use

$$\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^k \frac{f_l(r)}{r^l} = (x+iy)^k\left(\frac{1}{r}\frac{d}{dr}\right)^k \frac{f_l(r)}{r^l}, \quad (3.17)$$

$$\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^k (x-iy)^l = (-2)^k(-l)_k(x-iy)^{l-k}. \quad (3.18)$$

Here, $(-1)_k$ is a Pochhammer symbol. With the help of the theorem of Leibniz, the differentiation can be performed, and we obtain, for Eq. (3.16),

$$\mathscr{Y}_{l_1}^{l_1}(\nabla)F_{l_2}^{-l_2}(\mathbf{r}) = \frac{[(2l_1+1)!(2l_2+1)!]^{1/2}}{4\pi\,2^{l_2}\,l_1!l_2!}\sum_{k\geqslant 0}\frac{(-l_1)_k(-l_2)_{l_1-k}}{2^k k!}(x+iy)^k(x-iy)^{l_2-l_1-k}\left(\frac{1}{r}\frac{d}{dr}\right)^k\frac{f_{l_2}(r)}{r^{l_2}}. \quad (3.19)$$

In the next step, we express $(x+iy)^k$ and $(x-iy)^{l_2-l_1-k}$ in terms of solid harmonics according to Eq. (3.15). Then we couple the two solid harmonics according to

$$\mathscr{Y}_{l_1}^{m_1}(\mathbf{r})\,\mathscr{Y}_{l_2}^{m_2}(\mathbf{r}) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\langle l m_1 + m_2 | l_1 m_1 | l_2 m_2\rangle\, r^{l_1+l_2-l}\,\mathscr{Y}_l^{m_1+m_2}(\mathbf{r}), \quad (3.20)$$

which is an immediate consequence of Eq. (2.7). Finally, we introduce the new summation variable $q = l_1 - k$ to obtain, for Eq. (3.19),

$$\mathscr{Y}_{l_1}^{l_1}(\nabla)F_{l_2}^{-l_2}(\mathbf{r}) = \sum_{q\geqslant 0}\left[\frac{(2l_1+1)!(2l_2+1)!}{(2l_1-2q+1)!(2l_2-2q+1)!}\right]^{1/2}\frac{r^{l_1+l_2-2q}}{(-2)^q q!}\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-q}\frac{f_{l_2}(r)}{r^{l_2}}$$
$$\times\sum_{l=|l_1-l_2|}^{l_1+l_2-2q}{}^{(2)}\langle l l_1 - l_2 | l_1 - q\, l_1 - q | l_2 - q\, q - l_2\rangle\, Y_l^{l_1-l_2}(\mathbf{r}/r). \quad (3.21)$$

In order to obtain a result of the same structure as Eq. (3.9), it is necessary to have the l-summation as the outer sum and the q-summation as the inner sum. The summation limits of the l-summation would then be $|l_1 - l_2|$ and $l_1 + l_2$. The limits of the q-summation follow directly from the triangle condition of angular momentum coupling, which yields

$$0 \leqslant q \leqslant (l_1 + l_2 - l)/2 = \Delta l. \quad (3.22)$$

With these summation limits, we obtain, for Eq. (3.21),

$$\mathscr{Y}_{l_1}^{l_1}(\nabla)F_{l_2}^{-l_2}(\mathbf{r}) = \sum_{l=|l_1-l_2|}^{l_1+l_2}{}^{(2)} Y_l^{l_1-l_2}(\mathbf{r}/r) \times \sum_{q=0}^{\Delta l}\left[\frac{(2l_1+1)!(2l_2+1)!}{(2l_1-2q+1)!(2l_2-2q+1)!}\right]^{1/2}\langle ll_1-l_2|l_1-ql_1-q|l_2-qq-l_2\rangle \times\frac{r^{l_1+l_2-2q}}{(-2)^q q!}\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-q}\frac{f_{l_2}(r)}{r^{l_2}}. \tag{3.23}$$

On the other hand, if we set $m_1 = l_1$ and $m_2 = -l_2$ in Eq. (3.9), we obtain

$$\mathscr{Y}_{l_1}^{l_1}(\nabla)F_{l_2}^{-l_2}(\mathbf{r}) = \sum_{l=|l_1-l_2|}^{l_1+l_2}{}^{(2)}\langle ll_1-l_2|l_1l_1|l_2-l_2\rangle\,\gamma_{l_1l_2}^{l}(r)\,Y_l^{l_1-l_2}(\mathbf{r}/r). \tag{3.24}$$

Comparison of Eqs. (3.23) and (3.24) yields the following relationship which clearly demonstrates the group-theoretical origin of the numerical coefficients that occur in the q-summation:

$$\gamma_{l_1l_2}^{l}(r) = \sum_{q=0}^{\Delta l}\left[\frac{(2l_1+1)!(2l_2+1)!}{(2l_1-2q+1)!(2l_2-2q+1)!}\right]^{1/2}\frac{\langle ll_1-l_2|l_1-ql_1-q|l_2-qq-l_2\rangle}{\langle ll_1-l_2|l_1l_1|l_2-l_2\rangle}\frac{r^{l_1+l_2-2q}}{(-2)^q q!}\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-q}\frac{f_{l_2}(r)}{r^{l_2}}. \tag{3.25}$$

In the next step, we express the quotient of Gaunt coefficients in terms of $3jm$-symbols according to Eq. (2.6). We obtain

$$\gamma_{l_1l_2}^{l}(r) = \sum_{q=0}^{\Delta l}\left[\frac{(2l_1)!(2l_2)!}{(2l_1-2q)!(2l_2-2q)!}\right]^{1/2}\frac{\begin{pmatrix} l_1-q & l_2-q & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_1-q & l_2-q & l\\ l_1-q & q-l_2 & l_2-l_1\end{pmatrix}}{\begin{pmatrix} l_1 & l_2 & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_1 & l_2 & l\\ l_1 & -l_2 & l_2-l_1\end{pmatrix}}\frac{r^{l_1+l_2-2q}}{(-2)^q q!}\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-q}\frac{f_{l_2}(r)}{r^{l_2}} \tag{3.26}$$

Fortunately, all $3jm$-symbols occurring here can be expressed in closed form[26]

$$\begin{pmatrix} j_1 & j_2 & j\\ 0 & 0 & 0\end{pmatrix} = (-1)^{(j_1+j_2+j)/2}\left[\frac{(j_1+j_2+j)!(j_1-j_2+j)!(j_2-j_1+j)!}{(j_1+j_2+j+1)!}\right]^{1/2} \times\frac{((j_1+j_2+j)/2)!}{((j_1+j_2-j)/2)!((j_1-j_2+j)/2)!((j_2-j_1+j)/2)!}, \tag{3.27}$$

$$\begin{pmatrix} j_1 & j_2 & j\\ j_1 & -j_1-m & m\end{pmatrix} = (-1)^{j_2-j_1+m}\times\left[\frac{(2j_1)!(j_2-j_1+j)!(j_1+j_2+m)!(j-m)!}{(j_1+j_2+j+1)!(j_1-j_2+j)!(j_1+j_2-j)!(j_2-j_1-m)!(j+m)!}\right]. \tag{3.28}$$

If we insert these expressions into Eq. (3.26), we find that most terms cancel. After some algebraic manipulations we finally obtain, where Δl and $\sigma(l)$ are defined in Eq. (2.9),

$$\gamma_{l_1l_2}^{l}(r) = \sum_{q=0}^{\Delta l}\frac{(-\Delta l)_q(-\sigma(l)-1/2)_q}{q!}\,2^q\,r^{l_1+l_2-2q}\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-q}\frac{f_{l_2}(r)}{r^{l_2}}. \tag{3.29}$$

This representation of the function $\gamma_{l_1l_2}^{l}(r)$ is much more compact than the equivalent expression for the function $g_{l_1l_2}^{l}$ derived by Bayman.[27] We started from Eq. (3.9) which contains Gaunt coefficients, whereas Bayman started from Eq. (3.7) which contains Clebsch–Gordan coefficients. Hence the introduction of Gaunt coefficients instead of Clebsch–Gordan coefficients leads to a substantial simplification of the numerical coefficients and to an improved applicability of the result.

IV. APPLICATION OF THE SPHERICAL TENSOR GRADIENT—FOURIER TRANSFORM METHOD

Fourier transformation can advantageously be used to derive new representations for the function $\gamma_{l_1l_2}^{l}(r)$ defined in Eq. (3.9) because a differential operator is transformed into a multiplicative operator which usually can be handled much more easily. Hence in this section, we shall require that the following two integral representations exist:

$$\bar{F}_l^m(\mathbf{p}) = (2\pi)^{-3/2}\int e^{-i\mathbf{p}\cdot\mathbf{r}}F_l^m(\mathbf{r})d^3\mathbf{r}, \tag{4.1}$$

$$F_l^m(\mathbf{r}) = (2\pi)^{-3/2}\int e^{i\mathbf{r}\cdot\mathbf{p}}\bar{F}_l^m(\mathbf{p})d^3\mathbf{p}. \tag{4.2}$$

We now use the Rayleigh expansion of a plane wave Eq. (2.12) to express the function $\bar{F}_l^m(p)$ as a spherical harmonic multiplied by a radial integral

$$\bar{F}_l^m(\mathbf{p}) = \bar{f}_l(p)\,Y_l^m(\mathbf{p}/p), \tag{4.3}$$

$$\bar{f}_l(p) = (-i)^l p^{-1/2}\int_0^\infty r^{3/2}J_{l+1/2}(pr)f_l(r)\,dr. \tag{4.4}$$

If we insert these relationships into Eq. (4.2), we obtain an integral representation for the radial function $f_l(r)$:

$$f_l(r) = i^l r^{-1/2}\int_0^\infty p^{3/2}J_{l+1/2}(rp)\bar{f}_l(p)\,dp. \tag{4.5}$$

By similar means, we can derive an integral representation for the function $\gamma_{l_1l_2}^{l}(r)$. We use

$$\mathscr{Y}_l^m(\nabla)\,e^{i\mathbf{r}\cdot\mathbf{p}} = \mathscr{Y}_l^m(i\mathbf{p})\,e^{i\mathbf{r}\cdot\mathbf{p}} \tag{4.6}$$

together with the Rayleigh expansion Eq. (2.12) and the coupling rule of two spherical harmonics Eq. (2.7) to obtain

$$\mathscr{Y}_{l_1}^{m_1}(\nabla)\,F_{l_2}^{m_2}(\mathbf{r}) = (2\pi)^{-3/2}\int e^{i\mathbf{r}\cdot\mathbf{p}}\,\mathscr{Y}_{l_1}^{m_1}(i\mathbf{p})\,\bar{F}_{l_2}^{m_2}(\mathbf{p})\,d^3\mathbf{p}$$
$$= \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\langle lm_1+m_2|l_1m_1|l_2m_2\rangle \times i^{l+l_1}\,Y_l^{m_1+m_2}(\mathbf{r}/r) \times r^{-1/2}\int_0^\infty p^{l_1+3/2}J_{l+1/2}(rp)\bar{f}_{l_2}(p)\,dp\,. \quad (4.7)$$

If we compare Eqs. (3.9) and (4.7), we immediately obtain an integral representation for the function $\gamma_{l_1l_2}^l(r)$:

$$\gamma_{l_1l_2}^l(r) = i^{l+l_1}r^{-1/2}\int_0^\infty p^{l_1+3/2}J_{l+1/2}(rp)\bar{f}_{l_2}(p)\,dp\,. \quad (4.8)$$

With the help of the integral representations (4.5) and (4.8), we want to derive new differential operators which yield $\gamma_{l_1l_2}^l(r)$ when applied to $f_{l_2}(r)$. The differential operators we are looking for have to transform $p^{3/2}J_{l_2+1/2}(rp)$ into $p^{l_1+3/2}J_{l+1/2}(rp)$. As we shall show in this section, this can be accomplished by a suitable application of known differential properties of the Bessel functions of the first kind. We use the well-known relationships

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m z^\nu J_\nu(z) = z^{\nu-m}J_{\nu-m}(z)\,, \quad (4.9)$$

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m z^{-\nu}J_\nu(z) = (-1)^m z^{-\nu-m}J_{\nu+m}(z)\,, \quad (4.10)$$

to obtain immediately

$$\left(\frac{1}{x}\frac{d}{dx}\right)^m x^\nu J_\nu(xy) = y^m x^{\nu-m}J_{\nu-m}(xy)\,, \quad (4.11)$$

$$\left(\frac{1}{x}\frac{d}{dx}\right)^m x^{-\nu}J_\nu(xy) = (-1)^m\,y^m x^{-\nu-m}J_{\nu+m}(xy)\,. \quad (4.12)$$

These relationships can also be combined to give

$$\left(\frac{1}{x}\frac{d}{dx}\right)^m x^{2m-2\nu}\left(\frac{1}{x}\frac{d}{dx}\right)^m x^\nu J_\nu(xy) = (-1)^m\,y^{2m}x^{-\nu}J_\nu(xy)\,, \quad (4.13)$$

$$\left(\frac{1}{x}\frac{d}{dx}\right)^m x^{2\nu+2m}\left(\frac{1}{x}\frac{d}{dx}\right)^m x^{-\nu}J_\nu(xy) = (-1)^m\,y^{2m}x^\nu J_\nu(xy)\,. \quad (4.14)$$

By a suitable combination of these differential relations, we can derive the following differential operators which connect the functions $f_{l_2}(r)$ and $\gamma_{l_1l_2}^l(r)$:

$$\gamma_{l_1l_2}^l(r) = r^{-l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l} r^{l_1+l_2+l+1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l_2}\frac{f_{l_2}(r)}{r^{l_2}}\,, \quad (4.15)$$

$$\gamma_{l_1l_2}^l(r) = r^l\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l_2} r^{l_1-l_2-l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l} r^{l_2+1}f_{l_2}(r)\,, \quad (4.16)$$

$$\gamma_{l_1l_2}^l(r) = r^{-l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l_2} r^{l_1-l_2+3l+1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l_2} r^{2l-1}\times\left(\frac{1}{r}\frac{d}{dr}\right)^{l_2-l} r^{l_2+1}f_{l_2}(r)\,, \quad (4.17)$$

$$\gamma_{l_1l_2}^l(r) = r^l\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l} r^{l_1+l_2-3l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l} r^{2l+1}\times\left(\frac{1}{r}\frac{d}{dr}\right)^{l-l_2}\frac{f_{l_2}(r)}{r^{l_2}}\,. \quad (4.18)$$

It should be noted that the differential operator in Eq. (4.17) is meaningful only if $l_2 \geqslant l$ holds. Analogously, Eq. (4.18) requires $l \geqslant l_2$. The symbols Δl and Δl_2 were defined in Eq. (2.9).

These new representations for the function $\gamma_{l_1l_2}^l(r)$ seem to differ significantly from Eq. (3.29) which was derived by direct differentiation. Nevertheless, their equivalence can be proved quite easily. As an example we shall now prove the equivalence of Eqs. (3.29) and (4.16). If we combine Eq. (3.13) and the theorem of Leibniz we obtain, after some algebraic manipulations,

$$\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l_2} r^{l_1-l_2-l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l} r^{l_2+1}f_{l_2}(r) = \sum_{s=0}^{\Delta l_2}\sum_{t=0}^{l_1-s}(-1)^t \times 2^{s+t}\frac{(-\Delta l_2)_s(\Delta l_1+1/2)_s(l_1-s)!(-l_2-1/2)_t}{(l_1-s-t)!s!t!} \times r^{l_1+l_2-2s-2t-l}\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-s-t}\frac{f_{l_2}(r)}{r^{l_2}}\,. \quad (4.19)$$

We now introduce the new summation variable $q = s+t$ and obtain, after an elimination of t and some manipulations with Pochhammer symbols,

$$\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l_1} r^{l_1-l_2-l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l} r^{l_2+1}f_{l_2}(r) = \sum_{q\geqslant 0}\frac{(-l_2-1/2)_q(-l_1)_q}{q!} \times 2^q r^{l_1+l_2-l-2q}\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-q}\frac{f_{l_2}(r)}{r^{l_2}} \times {}_3F_2(-q,-\Delta l_2,\Delta l_1+1/2;-l_1,l_2-q+3/2;1)\,. \quad (4.20)$$

The generalized hypergeometric series ${}_3F_2$ in Eq. (4.20) can be expressed in closed form with the help of the summation theorem of Saalschütz[28]

$${}_3F_2(a,b,c;d,e;1) = \frac{\Gamma(d)\Gamma(1+a-e)\Gamma(1+b-e)\Gamma(1+c-e)}{\Gamma(1-e)\Gamma(d-a)\Gamma(d-b)\Gamma(d-c)}\,, \quad (4.21)$$

which holds for terminating hypergeometric series ${}_3F_2$ whose parameters satisfy

$$a+b+c+1 = d+e\,. \quad (4.22)$$

This summation theorem yields, for the terminating hypergeometric series in Eq. (4.20),

$$
{}_3F_2(-q,-\Delta l_2,\Delta l_1+1/2;-l_1,l_2-q+3/2;1) = \frac{(-\Delta l)_q(-\sigma(l)-\frac{1}{2})_q}{(-l_1)_q(-l_2-\frac{1}{2})_q}. \tag{4.23}
$$

Inserting this expression into Eq. (4.20) shows that Eqs. (3.29) and (4.16) are indeed equivalent. The equivalence of the other representations for the functions $\gamma^l_{l_1l_2}(r)$ can be proved by the same technique. When we proved the equivalence of Eqs. (3.29) and (4.16), we found still another representation:

$$
\gamma^l_{l_1l_2}(r) = \sum_{s=0}^{\Delta l_2} 2^s \frac{(-\Delta l_2)_s(\Delta l_1+1/2)_s}{s!} r^{l_1-l_2-2s-1} \times\left(\frac{1}{r}\frac{d}{dr}\right)^{l_1-s} r^{l_2+1} f_{l_2}(r). \tag{4.24}
$$

Which one of the representations for $\gamma^l_{l_1l_2}(r)$ presented in this article or of the equivalent formulas of Santos[4] or Stuart[7] is best suited for practical applications cannot be decided without explicitly considering the functional form of $f_{l_2}(r)$. Nevertheless, we think that because of the large number of functions $f_{l_2}(r)$ which are of interest, it should be advantageous to have as many representations as possible available.

As the generalization of the spherical tensor gradient, the differential operator

$$
\nabla^{2n}\mathscr{Y}^m_l(\nabla) \tag{4.25}
$$

may be considered. It was used by Santos,[4] Rowe,[5] and Stuart[7] or, in the book of Brink and Satchler,[29] in connection with multipole expansions. If we apply this operator to a spherical tensor we may derive the following integral representation:

$$
\nabla^{2n}\mathscr{Y}^{m_1}_{l_1}(\nabla)F^{m_2}_{l_2}(\mathbf{r}) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle lm_1+m_2|l_1m_1|l_2m_2\rangle \times G^{nl}_{l_1l_2}(r)\,Y^{m_1+m_2}_l(\mathbf{r}/r), \tag{4.26}
$$

$$
G^{nl}_{l_1l_2}(r) = i^{l+l_1+2n}r^{-1/2}\int_0^\infty p^{2n+l_1+3/2}J_{l+1/2}(rp)\,\bar{f}_{l_2}(p)\,dp. \tag{4.27}
$$

For these radial functions $G^{nl}_{l_1l_2}(r)$, explicit expressions may be derived quite easily. For instance, combining Eqs. (4.13) and (4.15) yields

$$
G^{nl}_{l_1l_2}(r) = r^l\left(\frac{1}{r}\frac{d}{dr}\right)^n r^{2n-2l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^{n+\Delta l} r^{l_1+l_2+l+1} \times\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l_2}\frac{f_{l_2}(r)}{r^{l_2}}. \tag{4.28}
$$

Also, if we combine Eqs. (4.14) and (4.16),

$$
G^{nl}_{l_1l_2}(r) = r^{-l-1}\left(\frac{1}{r}\frac{d}{dr}\right)^n r^{2n+2l+1}\left(\frac{1}{r}\frac{d}{dr}\right)^{n+\Delta l_2} r^{l_1-l_2-l-1} \times\left(\frac{1}{r}\frac{d}{dr}\right)^{\Delta l} r^{l_2+1}f_{l_2}(r). \tag{4.29}
$$

V. SOME PROPERTIES OF B FUNCTIONS

In this section, we want to discuss those mathematical properties of reduced Bessel functions, defined in Eq. (2.14), and their anisotropic generalization, the so-called B-functions, defined in Eq. (2.17), which are needed for the representation of the spherical delta function δ^m_l in terms of B functions.

As can be seen from Eqs. (2.15) and (2.17), B functions have a relatively complicated analytical representation. Nevertheless, as we could show recently, the Fourier transform of a B function is of exceptional simplicity[30]:

$$
\bar{B}^m_{n,l}(\alpha,\mathbf{p}) = (2\pi)^{-3/2}\int e^{-i\mathbf{p}\cdot\mathbf{r}}B^m_{n,l}(\alpha,\mathbf{r})d^3\mathbf{r} = (2/\pi)^{1/2}\frac{\alpha^{2n+l-1}}{[\alpha^2+p^2]^{n+l+1}}\mathscr{Y}^m_l(-i\mathbf{p}). \tag{5.1}
$$

It seems that the Fourier transform of a B function is more compact than the Fourier transforms of all other exponentially declining functions. Hence the Fourier transform of a B function may be considered as a kind of basic function in momentum space. This also explains why so many expansions of exponentially declining functions in terms of B functions or, equivalently, in terms of reduced Bessel functions could be derived, for instance,[31,32]

$$
x^{n-1}e^{-x} = \sum_{p=p_{\min}}^{n}\frac{(-1)^{n-p}n!}{(2p-n)!(2n-2p)!}\hat{k}_{p-1/2}(x), \tag{5.2a}
$$

$$
p_{\min} = \begin{cases} n/2 & \text{if } n \text{ is even}, \\ (n+1)/2 & \text{if } n \text{ is odd}, \end{cases} \tag{5.2b}
$$

$$
\frac{e^{-x}}{x}L^{(\alpha)}_n(2x) = \sum_{t=0}^{n}\frac{(-2)^t\Gamma(n+\alpha+t+1)}{t!(n-t)!\Gamma(\alpha+2t+1)}\hat{k}_{t-1/2}(x), \tag{5.3}
$$

$$
e^{-x}L^{(\alpha)}_n(2x) = (2n+\alpha+1)\sum_{t=0}^{n}\frac{(-2)^t\Gamma(n+\alpha+t+1)}{t!(n-t)!\Gamma(\alpha+2t+2)} \times\hat{k}_{t+1/2}(x). \tag{5.4}
$$

Here, $L^{(\alpha)}_n$ is an associated Laguerre polynomial. It should, however, be emphasized that these expansions were not derived using Fourier transform techniques. Instead, they were obtained by a straightforward rearrangement of the polynomial part.

The application of the Laplacian ∇^2 to a B function can be expressed as[33]

$$
\alpha^{-2}\nabla^2B^m_{n,l}(\alpha,\mathbf{r}) = B^m_{n,l}(\alpha,\mathbf{r}) - B^m_{n-1,l}(\alpha,\mathbf{r}). \tag{5.5}
$$

Hence we see that the differential operator $1-\alpha^{-2}\nabla^2$, which is essentially the differential operator of the modified Helmholtz equation, can be viewed as a ladder operator of the B function,

$$
[1-\alpha^{-2}\nabla]\,B^m_{n,l}(\alpha,\mathbf{r}) = B^m_{n-1,l}(\alpha,\mathbf{r}). \tag{5.6}
$$

This relationship can also be derived immediately from the Fourier transform of a B function, Eq. (5.1), because in momentum space, the operator $1-\alpha^{-2}\nabla$ is transformed into $[\alpha^2+p^2]/\alpha^2$.

The repeated application of the Laplacian ∇^2 can also be expressed quite easily. We use the binomial theorem in connection with Eq. (5.6) to obtain

$$\alpha^{-2\nu}\nabla^{2\nu}B_{n,l}^{m}(\alpha,\mathbf{r})=\sum_{t=0}^{\nu}(-1)^{t}\binom{\nu}{t}B_{n-t,l}^{m}(\alpha,\mathbf{r}). \quad (5.7)$$

In momentum space, the spherical tensor gradient $\mathscr{Y}_l^m(\nabla)$ is replaced by the solid harmonic $\mathscr{Y}_l^m(i\mathbf{p})$. Hence, from the Fourier transform of a B function, Eq. (5.1), it may be deduced that the application of the spherical tensor gradient to a scalar B function yields a nonscalar B function,[34]

$$B_{n,l}^{m}(\alpha,\mathbf{r})=\frac{(4\pi)^{1/2}}{(-\alpha)^{l}}\mathscr{Y}_l^m(\nabla)\,B_{n+l,0}^{0}(\alpha,\mathbf{r}). \quad (5.8)$$

Of course, this result may also be derived with the help of Eq. (3.12).

The centerpiece of the theory of B functions has so far been the convolution theorem.[12,13] In the case of equal scaling parameters we have

$$\int B_{n_1,l_1}^{m_1}(\alpha,\mathbf{x}-\mathbf{y})B_{n_2,l_2}^{m_2}(\alpha,\mathbf{y})\,d^3\mathbf{y}$$
$$=\frac{4\pi}{\alpha^3}\sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\langle lm_1+m_2|l_1m_1|l_2m_2\rangle$$
$$\times\sum_{t=0}^{\Delta l}(-1)^{t}\binom{\Delta l}{t}B_{n_1+n_2+l_1+l_2-l-t+1,l}^{m_1+m_2}(\alpha,\mathbf{x}). \quad (5.9)$$

It is of some importance to note that Eq. (5.9) differs slightly from the form in which it was derived. In the original publications,[11,12] overlap integrals as they occur in quantum chemistry were considered, whereas here we consider convolution integrals. Overlap and convolution integrals are connected by

$$\int B_{n_1,l_1}^{m_1}(\alpha,\mathbf{x}-\mathbf{y})\,B_{n_2,l_2}^{m_2}(\alpha,\mathbf{y})\,d^3\mathbf{y}$$
$$=(-1)^{m_1+l_2}\int B_{n_1,l_1}^{-m_1^*}(\alpha,\mathbf{y})\,B_{n_2,l_2}^{m_2}(\alpha,\mathbf{y}-\mathbf{x})\,d^3\mathbf{y}. \quad (5.10)$$

The convolution theorems of B functions were originally derived with the help of an addition theorem.[11,12] However, as we could show recently,[9] these convolution theorems can be derived much more easily if one makes use of the fact that the convolution integral of two functions f and g can be represented as an inverse Fourier transform,[35]

$$\int f(\mathbf{x}-\mathbf{y})g(\mathbf{y})d^3\mathbf{y}=\int e^{i\mathbf{x}\cdot\mathbf{p}}\bar{f}(\mathbf{p})\bar{g}(\mathbf{p})d^3\mathbf{p}. \quad (5.11)$$

Here, $\bar{f}$ and $\bar{g}$ are the Fourier transforms of f and g according to Eq. (2.10). Hence the simplicity of the convolution theorems of B functions[11,12] is a direct consequence of the simple analytical structure of the Fourier transform of a B function, Eq. (5.1).

VI. THE REPRESENTATION OF THE SPHERICAL DELTA FUNCTION BY A *B* FUNCTION

In this section, we want to show how the spherical delta function

$$\delta_l^m(\mathbf{r})=\frac{(-1)^l}{(2l-1)!!}\mathscr{Y}_l^m(\nabla)\delta(\mathbf{r}) \quad (6.1)$$

may be represented by a B function. In this context it is advantageous to consider convolutions

$$\int f(\mathbf{x}-\mathbf{y})g(\mathbf{y})d^3\mathbf{y} \quad (6.2)$$

instead of ordinary integrals

$$\int f(\mathbf{x})g(\mathbf{x})d^3\mathbf{x}. \quad (6.3)$$

A convolution integral exists for a relatively large class of functions f and g. In particular, a convolution integral usually remains well defined if f or g are distributions, and sometimes even if both f and g are distributions. The existence of integrals like (6.3) is guaranteed only if much more restrictive conditions are imposed on f and g. An integral (6.3) need not exist if f or g is a distribution, and the integral of the product of two distributions is generally not defined.

As we already mentioned earlier, a B function

$$B_{n,l}^{m}(\alpha,\mathbf{r})=[2^{n+l}(n+l)!]^{-1}\hat{k}_{n-1/2}(\alpha r)\,\mathscr{Y}_l^m(\alpha\mathbf{r}) \quad (6.4)$$

is classically defined only if the inequality $n+l\geqslant 0$ holds. In this section, we want to analyze how the above definition of B functions can be extended to such values of n where $n+l<0$ holds, i.e., to those cases where $(n+l)!=\Gamma(n+l+1)$ in the denominator in Eq. (6.4) becomes singular. It is obvious that such objects as $B_{-l-n,l}^{m}$, $n=1,2,\ldots$, cannot be ordinary functions but have to be interpreted as distributions.

We shall show in the sequel that functionals containing B functions can be found that remain well defined even if the order n becomes negative and satisfies the inequality $n+l<0$. With the help of these functionals, the distributive B functions can be identified. Our analysis will, to a large extent, be based upon the convolution theorem of B functions Eq. (5.9) and upon the differential operator $1-\alpha^{-2}\nabla^2$ which acts as a lowering operator for B functions according to Eq. (5.6).

Let us first consider convolutions with the scalar function $B_{0,0}^{0}$ which essentially corresponds to the Yukawa potential $e^{-\alpha r}/r$ because of

$$B_{0,0}^{0}(\alpha,\mathbf{r})=(4\pi)^{-1/2}e^{-\alpha r}/\alpha r. \quad (6.5)$$

From Eq. (5.9), we then obtain

$$\int B_{0,0}^{0}(\alpha,\mathbf{x}-\mathbf{y})\,B_{n,l}^{m}(\alpha,\mathbf{y})d^3\mathbf{y}=(4\pi)^{1/2}\alpha^{-3}B_{n+1,l}^{m}(\alpha,\mathbf{r}). \quad (6.6)$$

The convolution of a B function with the function $B_{0,0}^{0}$ merely increases the order n by one. Accordingly, Eq. (6.6) defines a raising operator for B functions. The inverse operator is the differential operator $1-\alpha^{-2}\nabla^2$ because of Eq. (5.6). We now exploit the fact that the composition of the two ladder operators must yield the identity. Accordingly, we apply the differential operator $1-\alpha^{-2}\nabla^2$ to the convolution integral (6.6). We differentiate under the integral sign and obtain, with the help of Eq. (5.6),

$$\int [1-\alpha^{-2}\nabla_x^2]\, B_{0,0}^{0}(\alpha,\mathbf{x}-\mathbf{y}) B_{n,l}^{m}(\alpha,\mathbf{y}) d^3\mathbf{y}$$

$$= \int B_{-1,0}^{0}(\alpha,\mathbf{x}-\mathbf{y})\, B_{n,l}^{m}(\alpha,\mathbf{y}) d^3\mathbf{y}$$

$$= \frac{(4\pi)^{1/2}}{\alpha^3} B_{n,l}^{m}(\alpha,\mathbf{x}), \tag{6.7}$$

which obviously implies, with $\nabla_x = \nabla_{x-y}$,

$$[1-\alpha^{-2}\nabla^2]\, B_{0,0}^{0}(\alpha,\mathbf{x}) = B_{-1,0}^{0}(\alpha,\mathbf{x}) = \frac{(4\pi)^{1/2}}{\alpha^3}\delta(\mathbf{x}). \tag{6.8}$$

This result becomes much more transparent if we repeat our derivation in momentum space. However, in order to show that the above result is not restricted to B functions but that it is of a more general nature, we prefer to consider the convolution of $B_{0,0}^{0}$ with a relatively arbitrary function $f:\mathbb{R}^3 \rightarrow \mathbb{C}$. Concerning f, we only require that the Fourier integral (2.10) and (2.11) exist. With the help of Eqs. (5.1) and (5.11) we represent the convolution integral under consideration by an inverse Fourier integral, i.e.,

$$\int B_{0,0}^{0}(\alpha,\mathbf{x}-\mathbf{y}) f(\mathbf{y}) d^3\mathbf{y} = \int e^{i\mathbf{x}\cdot\mathbf{p}} \bar{B}_{0,0}^{0}(\alpha,\mathbf{p}) \bar{f}(\mathbf{p}) d^3\mathbf{p}$$

$$= \frac{\alpha^{-1}}{(2\pi^2)^{1/2}} \int \frac{e^{i\mathbf{x}\cdot\mathbf{p}}}{\alpha^2+p^2} \bar{f}(\mathbf{p}) d^3\mathbf{p}. \tag{6.9}$$

Here, $\bar{f}(\mathbf{p})$ is the Fourier transform of $f(\mathbf{x})$ according to Eq. (2.10). The application of the lowering operator $1-\alpha^{-2}\nabla^2$ then again leads to Eq. (6.8), if we differentiate under the integral sign and use Eq. (5.6),

$$\int [1-\alpha^{-2}\nabla_x^2]\, B_{0,0}^{0}(\alpha,\mathbf{x}-\mathbf{y}) f(\mathbf{y}) d^3\mathbf{y}$$

$$= \int B_{-1,0}^{0}(\alpha,\mathbf{x}-\mathbf{y}) f(\mathbf{y}) d^3\mathbf{y}$$

$$= \frac{(4\pi)^{1/2}}{\alpha^3} (2\pi)^{-3/2} \int e^{i\mathbf{x}\cdot\mathbf{p}} \bar{f}(\mathbf{p}) d^3\mathbf{p} = \frac{(4\pi)^{1/2}}{\alpha^3} f(\mathbf{x}). \tag{6.10}$$

Hence we see that the application of $1-\alpha^{-2}\nabla^2$, which corresponds to $(\alpha^2+p^2)/\alpha^2$, transforms the representation of the convolution integral (6.9) by an inverse Fourier integral into an integral representation for the function f.

So far, we applied some mathematical properties of B functions to find a new derivation of the well-known fact that the Yukawa potential $e^{-\alpha r}/r$ is the Green's function of the modified Helmholtz equation. However, our approach can easily be extended to nonscalar functions. For instance, we set $n_1 = -l_1$ in the convolution theorem (5.9) to obtain

$$\int B_{-l_1,l_1}^{m_1}(\alpha,\mathbf{x}-\mathbf{y})\, B_{n_2,l_2}^{m_2}(\alpha,\mathbf{y}) d^3\mathbf{y}$$

$$= \frac{4\pi}{\alpha^3} \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle l m_1 + m_2 | l_1 m_1 | l_2 m_2 \rangle$$

$$\times \sum_{t=0}^{\Delta l} (-1)^t \binom{\Delta l}{t} B_{n_2+l_2-l-t+1,l}^{m_1+m_2}(\alpha,\mathbf{x}). \tag{6.11}$$

Again applying the lowering operator $1-\alpha^{-2}\nabla^2$ yields a functional which is perfectly well defined for sufficiently large values of n_2 and l_2:

$$\int B_{-l_1-1,l_1}^{m_1}(\alpha,\mathbf{x}-\mathbf{y})\, B_{n_2,l_2}^{m_2}(\alpha,\mathbf{y}) d^3\mathbf{y}$$

$$= \frac{4\pi}{\alpha^3} \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle l m_1 + m_2 | l_1 m_1 | l_2 m_2 \rangle$$

$$\times \sum_{t=0}^{\Delta l} (-1)^t \binom{\Delta l}{t} B_{n_2+l_2-l-t,l}^{m_1+m_2}(\alpha,\mathbf{x}). \tag{6.12}$$

In order to identify this distribution, we consider the special case that the other B function is scalar, i.e., $l_2 = 0$. After a rearrangement of quantum numbers, we then obtain

$$\int B_{-l-1,l}^{m}(\alpha,\mathbf{x}-\mathbf{y})\, B_{n+l,0}^{0}(\alpha,\mathbf{y}) d^3\mathbf{y}$$

$$= ((4\pi)^{1/2}/\alpha^3)\, B_{n,l}^{m}(\alpha,\mathbf{x}). \tag{6.13}$$

For a scalar B function, the convolution with the distribution $B_{-l-1,l}^{m}$ has essentially the same effect as the application of the spherical tensor gradient according to Eq. (5.8), i.e., it produces a nonscalar B function of rank l:

$$\int B_{-l-1,l}^{m}(\alpha,\mathbf{x}-\mathbf{y})\, B_{n+l,0}^{0}(\alpha,\mathbf{y})\, d^3\mathbf{y}$$

$$= (-1)^l (4\pi/\alpha^{l+3})\, \mathcal{Y}_l^m(\nabla)\, B_{n+l,0}^{0}(\alpha,\mathbf{x}). \tag{6.14}$$

Consequently, the distribution $B_{-l-1,l}^{m}$ must be proportional to the spherical delta function δ_l^m:

$$B_{-l-1,l}^{m}(\alpha,\mathbf{x}) = (-1)^l \frac{4\pi}{\alpha^{l+3}} \mathcal{Y}_l^m(\nabla)\delta(\mathbf{x})$$

$$= (2l-1)!!\, \frac{4\pi}{\alpha^{l+3}}\, \delta_l^m(\mathbf{x}). \tag{6.15}$$

In order to demonstrate the general nature of this result, we consider the convolution of the tempered distribution $B_{-l,l}^{m}$ with a relatively arbitrary function $f:\mathbb{R}^3 \rightarrow \mathbb{C}$:

$$\int B_{-l,l}^{m}(\alpha,\mathbf{x}-\mathbf{y}) f(\mathbf{y}) d^3\mathbf{y}. \tag{6.16}$$

Concerning f, we only require that the convolution integral as well as the Fourier integrals (2.10) and (2.11) exist. We could show recently that for the tempered distribution $B_{-l,l}^{m}$, the Fourier and inverse Fourier transform can be defined with the help of a suitable regularization[36] although these integrals may not exist in the sense of classical analysis. Accordingly, we can use Eqs. (5.1) and (5.11) to represent the convolution integral (6.16) as an inverse Fourier integral

$$\int B_{-l,l}^{m}(\alpha,\mathbf{x}-\mathbf{y}) f(\mathbf{y}) d^3\mathbf{y} = \int e^{i\mathbf{x}\cdot\mathbf{p}} \bar{B}_{-l,l}^{m}(\alpha,\mathbf{p}) \bar{f}(\mathbf{p}) d^3\mathbf{p}$$

$$= \frac{(2/\pi)^{1/2}}{\alpha^{l+1}} \int \frac{e^{i\mathbf{x}\cdot\mathbf{p}}}{\alpha^2+p^2} \mathcal{Y}_l^m(-i\mathbf{p}) \bar{f}(\mathbf{p}) d^3\mathbf{p}. \tag{6.17}$$

We again use the lowering operator $1-\alpha^{-2}\nabla$. Differentiating under the integral sign in connection with Eq. (5.6) then yields

$$\int B_{-l-1,l}^{m}(\alpha,\mathbf{x}-\mathbf{y}) f(\mathbf{y}) d^3\mathbf{y}$$

$$= \frac{(2/\pi)^{1/2}}{\alpha^{l+3}} \int e^{i\mathbf{x}\cdot\mathbf{p}}\, \mathcal{Y}_l^m(-i\mathbf{p}) \bar{f}(\mathbf{p}) d^3\mathbf{p}. \tag{6.18}$$

Finally, we use Eq. (4.6) to convert the Fourier integral in Eq. (6.18) into an integral representation for the function $f(\mathbf{x})$

onto which the spherical tensor gradient acts:

$$\int B^{m}_{-l-1,l}(\alpha,\mathbf{x}-\mathbf{y})f(\mathbf{y})d^3\mathbf{y}$$

$$=(-1)^l\frac{4\pi}{\alpha^{l+3}}\mathscr{Y}_l^m(\nabla)(2\pi)^{-3/2}\int e^{i\mathbf{x}\cdot\mathbf{p}}\bar{f}(\mathbf{p})d^3\mathbf{p}$$

$$=(-1)^l\frac{4\pi}{\alpha^{l+3}}\mathscr{Y}_l^m(\nabla)f(\mathbf{x})\,. \tag{6.19}$$

In view of these results, we can distinguish three different kinds of B functions according to the magnitude of the order $n\in\mathbb{Z}$.

(i) $n\geqslant 1$. These functions $B^m_{n,l}$ are absolutely summable and square summable, i.e., they belong to the space $L^1(\mathbb{R}^3)$ and $L^2(\mathbb{R}^3)$.

(ii) $-l\leqslant n\leqslant 0$. These functions are tempered distributions and are, in general, neither absolutely summable nor square summable. However, just as in case (i), they can be defined with the help of Eq. (6.4).

(iii) $n<-l$. These B functions are derivatives of the delta function. They can only be defined recursively with the help of Eq. (5.6). Accordingly, we obtain from Eq. (6.15), for $n=1,2,\ldots,$

$$B^m_{-l-n,l}(\alpha,\mathbf{x})=(-1)^l(4\pi/\alpha^{l+3})\times[1-\alpha^{-2}\nabla^2]^{n-1}\mathscr{Y}_l^m(\nabla)\delta(\mathbf{x})$$

$$=(2l-1)!!(4\pi/\alpha^{l+3})[1-\alpha^{-2}\nabla^2]^{n-1}\delta_l^m(\mathbf{x})\,. \tag{6.20}$$

In that context, it may be interesting to note that in contrast to coordinate space, no distinction concerning the magnitude of the order n is necessary in momentum space. The analytical representation of the Fourier transform Eq. (5.1) remains valid for all orders $n\in\mathbb{Z}$. Nevertheless, the Fourier transforms $\bar{B}^m_{n,l}$ can also be computed recursively. It is an easy matter to show that the functions $\bar{B}^m_{n,l}$ are unique solutions of the functional equations

$$\bar{B}^m_{n,l}(\alpha,\mathbf{p})=(\alpha^2/(\alpha^2+p^2))\,\bar{B}^m_{n-1,l}(\alpha,\mathbf{p})\,, \tag{6.21}$$

$$\bar{B}^m_{n,l}(\alpha,\mathbf{p})=((4\pi)^{1/2}/\alpha^l)\,\mathscr{Y}_l^m(-i\mathbf{p})\,\bar{B}^0_{n+l,0}(\alpha,\mathbf{p})\,, \tag{6.22}$$

$$\bar{B}^0_{-1,0}(\alpha,\mathbf{p})=\alpha^{-3}(2\pi^2)^{-1/2}\,. \tag{6.23}$$

These functional equations clearly show the intimate relationships between B functions, the differential operator of the modified Helmholtz equation, the spherical tensor gradient, and the delta function. These relationships also show that because of its simplicity, the Fourier transform of a B function may be considered to be a kind of basic function in momentum space.

From Eq. (6.22) we can immediately see that the application of the spherical tensor gradient to a nonscalar B function is equivalent to the coupling of two solid harmonics. Since a spherical tensor gradient and a solid harmonic transform identically under rotations, we must have the same coupling law

$$\mathscr{Y}_{l_1}^{m_1}(\nabla)\,\mathscr{Y}_{l_2}^{m_2}(\nabla)=\sum_{l=l_{\min}}^{l_{\max}\ (2)}\langle lm_1+m_2|l_1m_1|l_2m_2\rangle\times\nabla^{l_1+l_2-l}\,\mathscr{Y}_l^{m_1+m_2}(\nabla)\,. \tag{6.24}$$

Combining this result with Eqs. (5.7) and (5.8) yields

$$\mathscr{Y}_{l_1}^{m_1}(\nabla)\,B^{m_2}_{n_2,l_2}(\alpha,\mathbf{x})=(-\alpha)^{l_1}\sum_{l=l_{\min}}^{l_{\max}\ (2)}\langle lm_1+m_2|l_1m_1|l_2m_2\rangle\times\sum_{t=0}^{\Delta l}(-1)^t\binom{\Delta l}{t}B^{m_1+m_2}_{n_2+l_2-l-t,l}(\alpha,\mathbf{x})\,. \tag{6.25}$$

This relationship is structurally almost identical with the convolution theorem of B functions, Eq. (5.9). This similarity is easily understood if we take into consideration that we can also derive Eq. (6.25) by inserting Eq. (6.15) into the convolution integral (6.12).

If we compare Eq. (6.25) with the general results that were derived in Secs. III and IV, we see that the application of the spherical tensor gradient to a nonscalar B function leads to particularly simple expressions. Another advantage of Eq. (6.25) is that distributions which occur if $n_2+l_2-t<0$ holds cannot be overlooked, whereas the general expressions in Secs. III and IV require some caution. Hence particularly for exponentially declining functions, it may well be the most convenient approach to express the function under consideration as a linear combination of B functions and then apply the spherical tensor gradient according to Eq. (6.25).

VII. SUMMARY AND CONCLUSIONS

The spherical tensor gradient $\mathscr{Y}_l^m(\nabla)$ is a differential operator which transforms under rotations like an irreducible spherical tensor of rank l. Therefore we can use the well-known angular momentum coupling rules if we apply the spherical tensor gradient to a function $F_{l'}^{m'}(\mathbf{r})$, i.e., to a function which also transforms under rotations like an irreducible spherical tensor. With the help of angular momentum algebra, the result can be represented in terms of radial functions, Clebsch–Gordan coefficients, and spherical harmonics. The only quantities in this representation which depend upon the special nature of the function $F_{l'}^{m'}(\mathbf{r})$ and are not completely determined by the rules of angular momentum coupling are the radial functions. Hence, one has to find differential operators which when applied to the radial part of $F_{l'}^{m'}(\mathbf{r})$ yield the radial functions representing the product $\mathscr{Y}_l^m(\nabla)\,F_{l'}^{m'}(\mathbf{r})$.

Different methods for the derivation of such differential operators are discussed in this article. One method which was introduced by Bayman[6] exploits the fact that the solid harmonics $\mathscr{Y}_{l'}^{l'}(\mathbf{r})$ have a particularly convenient form. Therefore it is relatively easy to find a closed form representation for the special products $\mathscr{Y}_l^l(\nabla)\,F_{l'}^{l'}(\mathbf{r})$. We showed that the result of Bayman[27] can be simplified considerably if the Clebsch–Gordan coefficients are replaced by Gaunt coefficients, because then some inconvenient numerical coefficients that occur in the differential operators can be absorbed in the Gaunt coefficients. The computation of the Gaunt coefficients even for high angular momentum quantum numbers poses no problems because a very fast and reliable program is available.[18]

We also used Fourier transforms to derive alternative representations for the differential operators. Fourier transformation has the advantage that it converts a differential operator into a multiplicative operator which usually can be handled much more easily. The differential operators which were obtained with the help of Fourier transforms differ considerably from the ones which were derived by direct differentiation. Nevertheless, their equivalence could be proved explicitly.

Closely related to the spherical tensor gradient is the so-called spherical delta function δ_l^m. In this article, convolution integrals with the spherical delta function were studied. We derived representations of the spherical delta functions in terms of B functions which may be considered as generalizations of the well-known fact that the Yukawa potential is the Green's function of the modified Helmholtz equation. With the help of these results, we could extend the definition of the function $B_{n,l}^m(\alpha,\mathbf{x})$ to all $n\in\mathbb{Z}$. Classically, a B function is only defined if $n+l\geqslant 0$ holds. We are now able to identify the B functions, for which $n+l<0$ holds, with derivatives of the delta function, including the spherical delta function δ_l^m as a special case.

We investigated the spherical tensor gradient and the spherical delta function because we found that they are of particular importance in multicenter problems. As we shall show elsewhere the general results presented here can be used profitably in connection with addition theorems and multicenter integrals, which are of special importance in quantum mechanics of molecules.

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A useful formula for evaluating commutators

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We present the derivation of a useful formula for evaluating commutators of the form $[A,f(B)]$ and $[f(A),B]$, where the nested commutators $[A,[A,[\cdots[A\,[A,B]]\cdots]]]$ and $[[[\cdots[[A,B],B]\cdots],B],B]$ do not vanish in general. The use of this formula is illustrated by a simple example.

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I. INTRODUCTION

In many problems in modern physics, one is confronted with evaluating commutators of the form $[A,f(B)]$ and $[f(A),B]$ where A,B are operators with some or all of their nested commutators, $[A,[\cdots[A,[A,B]]\cdots]]$ and $[[\cdots[[A,B],B]\cdots],B]$ nonvanishing, and $f(B)$ and $f(A)$ are functions of the operators A and B. Below, we derive a general formula for evaluating these types of commutators when $f(B)$ and $f(A)$ can be written as a power series.

It is quite likely that this result is known to many people but the author has not seen it anywhere in the form presented here. Of course, some special cases of it appear in the literature,[1] e.g., for $[A, \exp B]$ which is certainly useful but by no means exhausts all the possibilities.

Before continuing, let me just state the result. For those who already know it or those who just want the answer, they need read no further.

$$[A,f(B)] = \sum_{n=1}^{\infty} \frac{1}{n!}(\partial_B^n f(B))[[\cdots[[A,B],B]\cdots],B],$$
$$[f(A),B] = \sum_{n=1}^{\infty} \frac{1}{n!}[A,[A\cdots[A,[A,B]]\cdots]](\partial_A^n f(A)), \tag{1.1}$$

where there are n nested commutators in the nth term. The usefulness of this formula arises from the fact that all the dependence on B (A) is to the left (right) of the commutators.

A note for mathematical purists: In (1.1) we have taken derivatives with respect to an operator. This is, in general, an ill-defined operation, but since $f(B)$ can be written as a power series in B, we need only define what we mean by ∂_B: $\partial_B B^n = nB^{n-1}$. Thus the only reason for using the notation ∂_B is that it reproduces the result we would get if B were a number.

In Sec. II we present a derivation of (1.1), and in Sec. III its use is illustrated by a simple example.

II. DERIVATION

Since we will deal with any $f(B)$ which can be written as a power series in B

$$f(B) = \sum_{n=0}^{\infty} a_n B^n, \tag{2.1}$$

we must first evaluate $[A,B^n]$. The result, which is proven below, is

$$[A,B^n] = \sum_{m=0}^{n-1} B^m C_{n-m}(A,B)\binom{n}{m}, \tag{2.2}$$

where $\binom{n}{m}$ are the standard binomial coefficients

$$\binom{n}{m} = \frac{n!}{m!(n-m)!}, \tag{2.3}$$

and $C_l(A,B)$ is given by

$$C_1(A,B) = [A,B],$$
$$C_2(A,B) = [[A,B],B], \tag{2.4}$$
$$C_l(A,B) = [[\cdots[[A,B],B]\cdots],B].$$

That is, in $C_l(A,B)$ there are l nested commutators. Usually, we will write C_l and omit the dependence on A and B.

We will prove (2.2) by induction. For $n=1$, (2.2) gives

$$[A,B] = \sum_{n=0}^{0} B^m C_{1-m}\binom{n}{m} = C_1 = [A,B].$$

Now suppose that (2.2) holds for an arbitrary n. We have

$$[A,B^{n+1}] = [A,B^n]B + B^n C_1$$
$$= \sum_{m=0}^{n-1} B^m C_{n-m}\binom{n}{m}B + B^n C_1,$$

but $C_l B = C_{l+1} + BC_l$; thus

$$[A,B^{n+1}] = \sum_{m=0}^{n-1} B^m C_{n-m+1}\binom{n}{m} + \sum_{m=0}^{n-1} B^{m+1}C_{n-m}\binom{n}{m} + B^n C_1$$
$$= C_{n+1} + \sum_{m=0}^{n-2}\left[\binom{n}{m+1} + \binom{n}{m}\right]B^{m+1}C_{n-m} + (n+1)B^n C_1$$
$$= C_{n+1} + \sum_{m=0}^{n-2}\binom{n+1}{m+1}B^{m+1}C_{n-m} + (n+1)B^n C_1 = \sum_{m=0}^{n}\binom{n+1}{m}B^m C_{n+1-m}.$$

Thus it holds for $n+1$, and we have proven (2.2).

Below, we will need the form for arbitrary derivatives of $f(B)$. From (2.1), this is easily seen to be

$$\partial^l_B f(B) = \sum_{m=l}^{\infty} a_m \frac{m!}{(m-l)!} B^{m-l}. \tag{2.5}$$

We now have, combining (2.1) and (2.2),

$$[A,f(B)] = \sum_{n=1}^{\infty} \sum_{m=0}^{n-1} a_n B^m C_{n-m} \binom{n}{m},$$

but

$$\sum_{n=1}^{\infty} \sum_{m=0}^{n-1} M_{m,n} = \sum_{m=0}^{\infty} \sum_{n=m+1}^{\infty} M_{m,n}, \tag{2.6}$$

therefore

$$[A,f(B)] = \sum_{m=0}^{\infty} \sum_{n=m+1}^{\infty} a_n B^m C_{n-m} \binom{n}{m}.$$

Replacing m with $n-m$ gives

$$[A,f(B)] = \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} a_n B^{n-m} C_m \binom{n}{m}$$
$$= \sum_{m=1}^{\infty} (\partial^m_B f(B)) \frac{1}{m!} C_m,$$

which is (1.1).

In the same manner, we arrive at

$$[f(A),B] = \sum_{m=1}^{\infty} \tilde{C}_m(A,B) \frac{1}{m!} \partial^m_A f(A),$$

where

$$\tilde{C}_m(A,B) = [A,[A,[\cdots[A,[A,B]]\cdots]]].$$

III. EXAMPLE

We will consider the case where $f(B) = \exp B$, then $\partial^n_B f(B) = f(B)$, and we have

$$[A,\exp B] = \exp B \sum_{m=1}^{\infty} \frac{C_m}{m!}. \tag{3.1}$$

Consider

$$e^B A e^{-B} = A + e^B [A,e^{-B}]$$
$$= A + e^B \left(e^{-B} \sum_{m=1}^{\infty} \frac{C_m(A,-B)}{m!} \right)$$
$$= A + \sum_{m=1}^{\infty} \frac{\tilde{C}_m(A,B)}{m!},$$

which is the standard result.[1]

Now let us show that $\Lambda_\mu{}^\nu = (e^b)_\mu{}^\nu$, where $\Lambda_\mu{}^\nu$ is the Lorentz transformation generated by $\exp((i/2)M_{\mu\nu} b^{\mu\nu})$, an element of the Poincare group with $b_{\mu\nu} = -b_{\nu\mu}$. Consider the standard result.[2]

$$e^{(i/2)M_{\mu\nu} b^{\mu\nu}} P_\alpha\, e^{-(i/2)M_{\mu\nu} b^{\mu\nu}} = \Lambda_\alpha{}^\beta P_\beta.$$

Taking $P_\alpha = A$ and $M_{\mu\nu} b^{\mu\nu}/2 = B$, we have, using (1.1) or (3.1),

$$e^{(i/2)M_{\mu\nu} b^{\mu\nu}} P_\alpha\, e^{-(i/2)M_{\mu\nu} b^{\mu\nu}}$$
$$= P_\alpha + \sum_{m=1}^{\infty} \frac{(-i)^m}{m!} C_m(P_\alpha, M_{\mu\nu} b^{\mu\nu}),$$

but

$$[P_\alpha, M_{\mu\nu} b^{\mu\nu}/2] = i b_\alpha{}^\beta P_\beta,$$

and thus

$$C_m(P_\alpha, M_{\mu\nu} b^{\mu\nu}) = (i)^m (b^m)_\alpha{}^\beta P_\beta,$$

where

$$(b^m)_\alpha{}^\beta = b_\alpha{}^{\nu_1} b_{\nu_1}{}^{\nu_2} b_{\nu_2}{}^{\nu_3} \cdots b_{\nu_{m-1}}{}^{\nu_m} b_{\nu_m}{}^\beta$$

with repeated indices summed. Thus

$$e^{(i/2)M_{\mu\nu} b^{\mu\nu}} P_\alpha e^{-(i/2)M_{\mu\nu} b^{\mu\nu}} = (e^b)_\alpha{}^\beta P_\beta, \tag{3.2}$$

and we have $\Lambda_\mu{}^\nu = (e^b)_\mu{}^\nu$.

[1] C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980), p. 70.

[2] L. Fonda and G. C. Ghirardi, *Symmetry Principles in Quantum Physics* (Marcel Dekker, New York, 1970), p. 276.

Dirac tensor distributions for moving submanifolds of R^n

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This paper considers nonclassical fields (tensor distributions) of the form $\tau\delta_{\Omega}$, where δ_{Ω} is the Dirac delta function for a moving p-dimensional submanifold of R^n ($0 \leqslant p \leqslant n$). The density τ is a classical (smooth), rank-k tensor field on R^{n+1}. The main result of the paper is the development of formulas for the distributional derivatives of such fields. The derivatives considered are the absolute differential (Levi-Civita connection), the covariant derivative along a given vector field, the divergence operator, the exterior differential, and the exterior codifferential. The resulting derived fields are shown to reflect the underlying geometry of the submanifold Ω as well as the nature of its motion. In the special case $p = n$, it is seen that the jump conditions on fields at the boundary of the region Ω arise naturally from the distributional calculus.

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I. INTRODUCTION

In a recent paper[1] it was shown how distribution theory (generalized functions) may be used to treat the topic of jump conditions on fields with either jump discontinuities or δ-function singularities on a moving surface. This topic was previously discussed in a paper of Costen,[2] which showed the applicability of this topic to certain aspects of electromagnetic field theory. Because there are numerous circumstances where fields occur with singularities on moving points, curves, or solid bodies (as, for instance, in the charge and current fields which occur as sources in the Maxwell equations[3]), it seems desirable to extend the treatment to submanifolds of all dimensions. At the same time it proves beneficial, for applications and geometric insight, to enlarge the dimension of the space in which the submanifolds move. The paper[4] of Estrada and Kanwal uses distributional methods to study the case of a hypersurface moving in n-dimensional space. Thus, I would like to extend herein their treatment to submanifolds of all dimensions and also to broaden their distributional calculus to include the standard differential operators from differential geometry.

The subject of this paper then is the study of Dirac tensor distributions $\tau\delta_{\Omega}$, where Ω is a moving p-dimensional submanifold of R^n ($0 \leqslant p \leqslant n$) and τ is a rank-k, smooth tensor field on R^{n+1}. In the case where τ is antisymmetric (a differential form), $\tau\delta_{\Omega}$ is known as a current (after de Rham). The definition and discussion of these distributions is given in Sec. II. The distributional derivatives considered are: the absolute differential ∇, the covariant derivative ∇_X along a vector field X, the divergence operator div, the exterior differential d, and the exterior codifferential d'. The calculation of the action of these operators D on $\tau\delta_{\Omega}$ is accomplished in a coordinate-free manner by using Theorem 1 from Sec. III and the transport theorem (from continuum mechanics). It is shown in Sec. IV that D applied to $\tau\delta_{\Omega}$ gives a nonclassical field of the form

$$D(\tau\delta_{\Omega}) = A\delta_{\partial\Omega} + B\delta_{\Omega} + \sum_{i=1}^{q} C_i\cdot\nabla_{\nu_i}(\cdot)\delta_{\Omega}. \qquad (1)$$

Here $\partial\Omega$ denotes the boundary of Ω and $\nu_1, ..., \nu_q$ are unit vector fields which are mutually orthogonal and normal to Ω at each point during the motion. The tensor densities A, B, $C_1, ..., C_q$ are intimately connected with the geometry and motion of Ω. As a corollary it is also shown in Sec. IV that if τ is a classical tensor field which is smooth except at the points on a moving $(n-1)$-dimensional submanifold Ω of R^n (hypersurface), then

$$D\{\tau\} = \{D\tau\} + ([\tau]\odot\nu)\delta_{\Omega}.$$

Here $\{\tau\}$ denotes the distribution determined by τ, ν is a vector field normal to Ω, $[\tau] = \tau_+ - \tau_-$ is the jump in τ across Ω in the direction ν and the product $\odot$ depends on the particular operator D chosen. Comments on the nature of the decomposition shown in Eq. (1) are presented in Sec. V.

Examples and applications of this work to field theory are numerous and extensive, some of which, in the limited form available at the time, were presented in the papers previously cited.[1,2,4] In a sequel[5] to this paper, I have presented applications of the distributional calculus for Dirac tensor distributions as developed here in its general form.

II. DEFINITIONS AND NOTATION

This section serves to outline some of the concepts and definitions which are needed in this paper. Unexplained concepts may be found in standard references on differential geometry and distribution theory.[6]

(*1*) *Submanifolds*: In the n-dimensional space R^n a p-dimensional submanifold Ω and its $(p-1)$-dimensional boundary $\partial\Omega$ are considered to be smooth and to be parametrized by maps $\alpha: U \to \Omega$ and $\lambda: I \to \partial\Omega$, where $U \subset R^p$ and $I \subset R^{p-1}$ are the parameter domains (more general situations can be reduced to this by using coordinate neighborhoods). It is assumed that, with α given, the boundary parametrization λ is coherently oriented with α.[7] One has that $\partial\alpha/\partial u_1, ..., \partial\alpha/\partial u_p$ are vector fields along Ω which form a basis for the tangent space at each point. Let $q = n - p$ and let $\nu_1, ..., \nu_q$ be unit vector fields along Ω which at each point are normal to Ω, mutually orthogonal to each other, and such that $\det(\partial\alpha/\partial u_1, ..., \partial\alpha/\partial u_p, \nu_1, ..., \nu_q) > 0$. This last expression denotes the determinant of the $n \times n$ matrix formed by using the indicated vectors as columns. The outward directed normal to $\partial\Omega$ is the unit vector field ν along and $\partial\Omega$ such that $\det(\partial\lambda/\partial s_1, ..., \partial\lambda/\partial s_{p-1}, \nu, \nu_1, ..., \nu_q) > 0$ on $\partial\Omega$. (The choice of terminology here is just for convenience of reference.) By a standard partition of unity argument one can extend $\nu_1, ..., \nu_q$, and ν to vector fields on all of R^n. Figures 1 and 2 illustrate these concepts for submanifolds of R^3.

(2) Content forms: With regard to the choice of frame $\nu_1, ..., \nu_q$ in the normal bundle, the content form for Ω is defined to be the differential p-form

$$\omega = i_{\nu_1} i_{\nu_2} \cdots i_{\nu_q}(\pi).$$

Here i_{ν_m} denotes the interior product operator (contraction with ν_m, and sometimes denoted by $\nu_m \lrcorner$) and π is a content form (volume form) for R^n. In a similar fashion the content form for $\partial\Omega$ is taken to be

$$\partial\omega = i_\nu i_{\nu_1} i_{\nu_2} \cdots i_{\nu_q}(\pi).$$

The integration of ω over Ω gives the content or measure of Ω (when it is finite):

$$\int_\Omega \omega = \int_{\alpha(U)} \omega = \int_U \alpha^*(\omega).$$

The last equation is the change of variables formula and $\alpha^*(\omega)$ is the pullback of ω by means of α, which in this case works out to be

$$\alpha^*(\omega) = \det\left(\frac{\partial\alpha}{\partial u_1}, ..., \frac{\partial\alpha}{\partial u_p}, \nu_1 ... \nu_q\right) \times du^1 \wedge du^2 \wedge \cdots \wedge du^p.$$

(3) The mean curvature normal: This is the normal vector field μ along Ω which is given by

$$\mu = \frac{1}{p} \sum_{m=1}^{q} \mu_m \nu_m,$$

where $\mu_m = -(\operatorname{div}(\nu_m) + \Sigma_{s=1}^q [\nu_m, \nu_s] \cdot \nu_s)$. The bracket $[\,,]$ is the Lie bracket and the dot is the dot product arising from the metric g. One can think of μ_s as the mean curvature of Ω relative to ν_s, and, in the case where $p = n-1$ and $q = 1$, μ_1/p gives the usual mean curvature for a hypersurface in R^n. Another interesting case is where $p = 1$ and $q = n-1$, so that Ω is a curve in R^n. Let l be a unit tangent vector to Ω and suppose that $l, \nu_1, \nu_2, ..., \nu_q$ is the distinguished Frenet frame along Ω. Then one can show that

$$\mu = \kappa_1 \nu_1,$$

where κ_1 is the first curvature of Ω. One also sees that when Ω is a point ($p = 0$), then $\mu = 0$ (by choosing the ν_i's to be constant) and that when Ω is n-dimensional, $\mu = 0$ by convention.

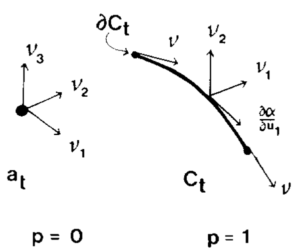

FIG. 1. Normal bundle frames $\{\nu_i\}$ for a moving point and moving curve.

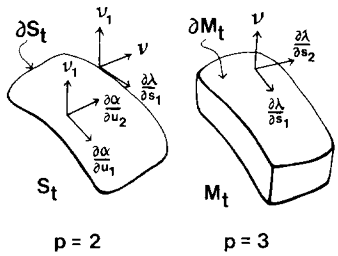

FIG. 2. Normal bundle frames $\{\nu_i\}$ for a moving surface and moving solid body.

(4) Kinematics: A motion of the submanifold Ω in R^n is modeled by means of the flow ϕ_t generated by a vector field V on R^n (V is thought of as a velocity vector field). One considers $\Omega_t \equiv \{\phi_t(x) | x \in \Omega\} = \phi_t(\Omega)$ as the submanifold into which Ω has deformed over the time interval t. Similar comments hold for $\partial\Omega_t = \phi_t(\partial\Omega)$. Parameterizations for Ω and $\partial\Omega$ are given by $\alpha_t \equiv \phi_t \circ \alpha$ and $\lambda_t \equiv \phi_t \circ \lambda$. One assumes also that the extension of the normal fields $\nu_1, ..., \nu_q, \nu$ along Ω and $\partial\Omega$ to all of R^n, as mentioned in (1) above, has been done so that $\nu_1, ..., \nu_q$ restricted to Ω_t is an orthonormal basis for the normal bundle to Ω_t and that ν restricted to $\partial\Omega$ is the outward directed normal.

(5) Tensor distributions: The tube in R^{n+1} swept out by the submanifold Ω moving in R^n is $\tilde{\Omega} = \{(\phi_t(x), t) | x \in \Omega, t \in R^1\}$, and the Dirac delta distribution for Ω is defined by

$$\langle \delta_{\tilde{\Omega}} | \psi \rangle = \int_{\tilde{\Omega}} \psi\omega = \int_R \left(\int_{\Omega_t} \psi\omega\right) dt = \int_R \left(\int_U \psi(\alpha_t(u), t) \alpha_t^*(\omega)\right) dt,$$

where ψ is a scalar field on R^{n+1} with compact support. If τ is a rank-k tensor field on R^{n+1}, then $\tau\delta_{\tilde{\Omega}}$ is the rank-k tensor distribution defined by

$$\langle \tau\delta_{\tilde{\Omega}} | \theta \rangle = \langle \delta_{\tilde{\Omega}} | \tau \cdot \theta \rangle.$$

Here θ is a rank-k tensor field on R^{n+1} with compact support.[8] The dot product above is defined more generally as follows: If σ is of rank $k + m$, than $(\tau \cdot \sigma)$ is the rank-m tensor field with components given by

$$(\tau \cdot \sigma)_{j_1 \cdots j_m} = \sum_{i_1 \cdots i_k} \tau_{i_1 \cdots i_k} \sigma^{i_1 \cdots i_k j_1 \cdots j_m}.$$

(The product in the other order, $\sigma \cdot \tau$, is defined in a similar but distinct fashion.) This, of course, relies on the metric which one uses on R^{n+1}. The results to be derived require a flat metric, and so I will assume that $\tilde{g} = \Sigma_{i=1}^{n+1} g_{ii}\, dx^i \otimes dx^i$ (Cartesian coordinates) with $g_{ii} = \pm 1$ for each i. The metric on R^n is taken to be $g = \Sigma_{i=1}^n g_{ii}\, dx^i \otimes dx^i$.

(6) Distributional derivatives: The extension of the differential operators from acting on classical fields to acting on distributions is achieved by means of duality and is designed to yield the customary results when restricted back to classical fields. If T is a tensor distribution (or current, where

appropriate), one defines

$$\langle \nabla T | \theta \rangle = -\langle T | \mathrm{div}(\theta) \rangle,$$
$$\langle \mathrm{div}(T) | \theta \rangle = -\langle T | \nabla \theta \rangle,$$
$$\langle \nabla_X T | \theta \rangle = \langle \nabla T | X \otimes \theta \rangle,$$
$$\langle dT | \theta \rangle = \langle T | d'\theta \rangle,$$
$$\langle d'T | \theta \rangle = \langle T | d\theta \rangle.$$

Here θ is a tensor field or differential form of appropriate rank and with compact support.

If θ is a vector field on R^{n+1}, one can decompose it into spatial and time components:

$$\theta = \vec{\theta} + \theta^{n+1} e_{n+1},$$

where $\vec{\theta} = \Sigma_{i=1}^{n} \theta^i e_i$ (Cartesian coordinates). Then if T is a scalar distribution on R^{n+1}, the spatial gradient of T is defined by

$$-\langle \vec{\nabla} T | \theta \rangle = \langle T | \mathrm{div}(\vec{\theta}) \rangle$$

Of special concern to the results of the paper are distributions of the form $C_i \cdot \nabla_{\nu_i}(\cdot)\delta_{\tilde{\Omega}}$, where C_i is a rank-k tensor field on R^{n+1} and ν_i is a normal vector field as mentioned in (1) above. The definition of such a distribution is

$$\langle C_i \cdot \nabla_{\nu_i}(\cdot)\delta_{\tilde{\Omega}} | \theta \rangle = \langle \delta_{\tilde{\Omega}} | C_i \cdot \nabla_{\nu_i}(\theta) \rangle.$$

III. THE TIME DERIVATIVE AND SPATIAL GRADIENT OF $\delta_{\tilde{\Omega}}$

In this section the calculations of $\partial(\delta_{\tilde{\Omega}})/\partial t$ and $\nabla(\delta_{\tilde{\Omega}})$ are presented. These results, while being special cases of the results presented in the next section, are derived here and used to prove the results there.

The first theorem allows me to derive all of the results in a coordinate-free manner which, I feel, is an improvement over previous methods. The theorem essentially gives (when $\psi = 1$) a calculation of the Lie derivative of the various content forms. Since in general $L_V = i_V d + d i_V$, the Lie derivative of the content form π for R^n is easy to calculate:

$$L_V \pi = d i_V \pi = \mathrm{div}(V)\pi.$$

Using Stokes' theorem, this gives the well-known divergence theorem

$$\int_\Omega L_V \pi = \int_{\partial\Omega} (V \cdot \nu)\, \partial\pi,$$

where Ω is an n-dimensional submanifold of R^n. A generalization of this is the following:

Theorem 1: Suppose that Ω is a p-dimensional submanifold of R^n with mean curvature normal μ, with content form $\omega = i_{\nu_1} \cdots i_{\nu_q}(\pi)$, and with content form $\partial\omega = i_\nu i_{\nu_1} \cdots i_{\nu_q}(\pi)$ for the boundary $\partial\Omega$. If V is any vector field and ψ any scalar field on R^n, then

$$\int_\Omega L_V(\psi\omega) = \int_{\partial\Omega} (V \cdot \nu)\psi\, \partial\omega - \int_\Omega p(V \cdot \mu)\psi\omega + \sum_{i=1}^{q} \int_\Omega (V \cdot \nu_i)(\nabla_{\nu_i}\psi)\omega. \tag{2}$$

Proof: The Lie derivative is expressible in the form $L_V = d i_V + i_V d$. Using this, the product rule for the exterior derivative d, and Stokes' theorem, one gets

$$\int_\Omega L_V(\psi\omega) = \int_\Omega [d i_V(\psi\omega) + i_V d(\psi\omega)]$$
$$= \int_{\partial\Omega} \psi\, i_V \omega + \int_\Omega \psi\, i_V d\omega + \int_\Omega i_V (d\psi \wedge \omega)$$
$$= A + B + C.$$

The rest of the proof consists of showing that the three terms A, B, C coincide with the three corresponding terms in Eq. (2).

(A) With regard to the parametrization λ of $\partial\Omega$ the differential form $i_V\omega$ pulls back to

$$\lambda^*(i_V\omega) = \det\left(\frac{\partial\lambda}{\partial s_1}, \ldots, \frac{\partial\lambda}{\partial s_{p-1}}, V, \nu_1, \ldots, \nu_q\right) \times ds^1\, ds^2 \cdots ds^{p-1}.$$

Expressing V in terms of the natural basis

$$V = a_1 \frac{\partial\lambda}{\partial s_1} + \cdots + a_{p-1} \frac{\partial\lambda}{\partial s_{p-1}} + b\nu + c_1\nu_1 + \cdots + c_q\nu_q,$$

the above determinant is seen to reduce to

$$b \det\left(\frac{\partial\lambda}{\partial s_1}, \ldots, \frac{\partial\lambda}{\partial s_{p-1}}, \nu, \nu_1, \ldots, \nu_q\right) = b\lambda^*(\partial\omega).$$

But $b = V \cdot \nu$ and so one sees that

$$\lambda^*[\psi i_V \omega] = \lambda^*[(V \cdot \nu)\psi\, \partial\omega],$$

which shows that the term A coincides with the first term in Eq. (2).

(B) To see that the term B coincides with the second term in Eq. (2), one takes the differential form

$$i_V d\omega = i_V d\, i_{\nu_1} \cdots i_{\nu_q} \pi$$

and simply commutes the operator d past $i_{\nu_1} \cdots i_{\nu_q}$. It is conceptually simpler to do this in two stages. First by viewing the identity $d i_a + i_a d = L_a$ as a commutation relation and using the fact that $d\pi = 0$, one arrives at

$$d\omega = \sum_{m=1}^{q} (-1)^{m-1} i_{\nu_1} \cdots L_{\nu_m} \cdots i_{\nu_q} \pi,$$

where in the mth term L_{ν_m} replaces i_{ν_m} in the product $i_{\nu_1} \cdots i_{\nu_q}$. Next, looking at the mth term of $i_V d\omega$, one can commute L_{ν_m} past $i_{\nu_{m+1}} \cdots i_{\nu_q}$ by using the commutation relation $L_a i_b - i_b L_a = i_{[a,b]}$. If one uses the facts that $L_a \pi = \mathrm{div}(a)\pi$ and that $i_a i_b \pi = -i_b i_a \pi$, then one arrives at the identity

$$i_V d\omega = \sum_{m=1}^{q} \mathrm{div}(\nu_m) i_{\nu_1} \cdots i_V \cdots i_{\nu_q} \pi + \sum_{m=1}^{q-1} \sum_{s=m+1}^{q} i_{\nu_1} \cdots i_V \cdots i_{[\nu_m,\nu_s]} \cdots i_{\nu_q} \pi \tag{3}$$

The notation here is that, in the mth term of the first summation, i_V replaces i_{ν_m} in the product $i_{\nu_1} \cdots i_{\nu_q}$ and, in the m, s term in the double summation, i_V replaces i_{ν_m} and $i_{[\nu_m,\nu_s]}$ replaces i_{ν_s} in the product $i_{\nu_1} \cdots i_{\nu_q}$. Finally, one needs to evaluate the restriction of $i_V d\omega$ to the submanifold Ω. For this, suppose that in the natural basis

$$V=\sum_{i=1}^{p} a_i \frac{\partial\alpha}{\partial u_i} + \sum_{i=1}^{q} N_i \nu_i,$$

$$[\nu_m,\nu_s] = \sum_{i=1}^{p} b_i \frac{\partial\alpha}{\partial u_i} + \sum_{i=1}^{q} A^{\,i}_{\,ms}\nu_i.$$

Then, of course,

$$N_i = V\cdot\nu_i \quad \text{amd} \quad A^{\,i}_{\,ms} = [\nu_m,\nu_s]\cdot\nu_i.$$

Evaluating the individual terms in Eq. (3) gives

$$\begin{aligned}
&\alpha^*(i_{\nu_1}\cdots i_V\cdots i_{\nu_q}\pi)\\
&\quad=\det\left(\frac{\partial\alpha}{\partial u_1},\ldots,\frac{\partial\alpha}{\partial u_p},\nu_1,\ldots,V,\cdots\nu_q\right)du^1\cdots du^p\\
&\quad=N_m\det\left(\frac{\partial\alpha}{\partial u_1}\cdots,\frac{\partial\alpha}{\partial u_p},\nu_1,\cdots\nu_m,\cdots\nu_q\right)du^1\cdots du^p\\
&\quad=N_m\alpha^*(\omega),
\end{aligned}$$

where i_V and V occur in the mth positions. Also,

$$\begin{aligned}
&\alpha^*(i_{\nu_1}\cdots i_V\cdots i_{[\nu_m,\nu_s]}\cdots i_{\nu_q}\pi)\\
&\quad=\det\left(\frac{\partial\alpha}{\partial u_1},\ldots,\frac{\partial\alpha}{\partial u_p},\nu_1,\ldots,V,\ldots,[\nu_m,\nu_s],\cdots\nu_q\right)\\
&\qquad\times du^1\cdots du^p\\
&\quad=[N_m A^{\,s}_{\,ms}-N_s A^{\,m}_{\,ms}]\alpha^*(\omega).
\end{aligned}$$

In the above expression i_V occurs in the mth position, and $i_{[\nu_m,\nu_s]}$ occurs in the sth position. Using these calculations, one gets that

$$\begin{aligned}
\alpha^*(i_V d\omega)&=\alpha^*\Bigg(\Bigg[\sum_{m=1}^{q}N_m\operatorname{div}(\nu_m)\\
&\qquad+\sum_{m=1}^{q}\sum_{s=m+1}^{q}(N_m A^{\,s}_{\,ms}-N_s A^{\,m}_{\,ms})\Bigg]\omega\Bigg)\\
&=-p\alpha^*((V\cdot\mu)\omega).
\end{aligned}$$

The last equation follows from the definition of the mean curvature normal and the fact that the double summation above reduces to

$$\sum_{m=1}^{q}N_m\sum_{s=1}^{q}A^{\,s}_{\,ms}.$$

(C) In the expression

$$i_V(d\psi\wedge\omega)=i_V d\psi\wedge(i_{\nu_1}\cdots i_{\nu_q}\pi),$$

one can commute $d\psi$ past $i_{\nu_1}\cdots i_{\nu_q}$ by using the identity

$$d\psi\wedge i_a\sigma=(\nabla_a\psi)\sigma-i_a(d\psi\wedge\sigma)$$

which holds for any differential form σ. One then arrives at

$$i_V(d\psi\wedge\omega)=\sum_{m=1}^{q}(\nabla_{\nu_m}\psi)i_{\nu_1}\cdots i_V\cdots i_{\nu_q}\pi,$$

where in the mth term i_V replaces i_{ν_m} in the product $i_{\nu_1}\cdots i_{\nu_q}$. Using now an argument similar to that for part (B), one sees that

$$\alpha^*[i_V(d\psi\wedge\omega)]=\alpha^*\left(\left[\sum_{m=1}^{q}(\nabla_{\nu_m}\psi)(V\cdot\nu_m)\right]\omega\right),$$

which is what was to be shown.

Theorem 1 and its proof contain many results which are of importance in their own right. For the purpose of this paper, however, Theorem 1 together with the following theorem are instrumental in the calculation of $\partial/\partial t(\tau\delta_{\bar\Omega})$ and $\vec\nabla(\tau\delta_{\bar\Omega})$. The following theorem arises in kinematics and the proof of it together with other applications may be found in a recent paper.[9]

Theorem 2 (transport theorem): Suppose that ϕ_t is the flow generated by a vector field V on R^n. If ψ is a scalar field on R^{n+1}, ω a differential p-form on R^n, and Ω a p-dimensional submanifold of R^n, then

$$\frac{d}{dt}\int_{\phi_t(\Omega)}\psi\omega=\int_{\phi_t(\Omega)}\left[\frac{\partial\psi}{\partial t}\omega+L_V(\psi\omega)\right].$$

While in general the transport theorem applies to any p-form ω, I want now to apply it to the case where ω is a content form for Ω. One can easily see then how the last two theorems combine to give:

Theorem 3: The Dirac delta distribution $\delta_{\bar\Omega}$ for a moving p-dimensional submanifold Ω of R^n has time derivative given by

$$\frac{\partial}{\partial t}(\delta_{\bar\Omega})=N\delta_{\partial\bar\Omega}-pM\delta_{\bar\Omega}+\sum_i N_i\nabla_{\nu_i}(\cdot)\delta_{\bar\Omega}.$$

Here

$$N=V\cdot\nu,\quad M=V\cdot\mu,\quad\text{and } N_i=V\cdot\nu_i$$

are the velocities in the various normal directions.

Proof: Suppose that ψ is a scalar field on R^{n+1} with compact support. Then, using the definitions and the transport theorem, one gets that

$$\begin{aligned}
\left\langle\frac{\partial}{\partial t}\delta_{\bar\Omega}\,\middle|\,\psi\right\rangle&=-\left\langle\delta_{\bar\Omega}\,\middle|\,\frac{\partial\psi}{\partial t}\right\rangle=-\int_R\left(\int_{\Omega_t}\frac{\partial\psi}{\partial t}\omega\right)dt\\
&=-\int_R\frac{d}{dt}\left(\int_{\Omega_t}\psi\omega\right)dt\\
&\quad+\int_R\left[\int_{\Omega_t}L_V(\psi\omega)\right]dt.
\end{aligned}$$

Now the first term in this last equation is zero since it is equal to

$$\begin{aligned}
&-\lim_{s\to\infty}\int_{-s}^{s}\frac{d}{dt}\left(\int_{\Omega_t}\psi\omega\right)dt\\
&\quad=-\lim_{s\to\infty}\left[\int_{\Omega_s}\psi(\cdot,s)\omega-\int_{\Omega_{(-s)}}\psi(\cdot,-s)\omega\right].
\end{aligned}\tag{4}$$

But since ψ has compact support, there is an $r>0$ such that $\psi(x,s)=0$ for every $x\in R^n$ and every s with $|s|>r$, and consequently both the integrals in (4) are zero for s large. With this established, the result of the theorem follows directly from Theorem 1 and the arbitrariness of ψ.

Theorem 4: The Dirac delta function $\delta_{\bar\Omega}$ has spatial gradient given by

$$\vec\nabla(\delta_{\bar\Omega})=-\nu\delta_{\partial\bar\Omega}+p\,\mu\delta_{\bar\Omega}-\sum_i\nu_i\cdot\nabla_{\nu_i}(\cdot)\delta_{\bar\Omega}.$$

Proof: Suppose θ is a vector field on R^{n+1} with compact support and with no time component ($\theta=\vec\theta$). Then from the definition of $\overrightarrow{\nabla}$ one has

$$\langle\vec{\nabla}(\delta_{\tilde\Omega})|\theta\rangle = -\langle\delta_{\tilde\Omega}|\operatorname{div}(\theta)\rangle$$
$$= -\int_R\left[\int_{\Omega_t}\operatorname{div}(\theta)\omega\right]dt. \tag{5}$$

Next note that

$$\operatorname{div}(\theta)\omega = \operatorname{div}(\theta)i_{\nu_1}\cdots i_{\nu_q}\pi$$
$$= i_{\nu_1}\cdots i_{\nu_q}(\operatorname{div}\theta\,\pi)$$
$$= i_{\nu_1}\cdots i_{\nu_q}L_\theta\pi$$
$$= L_\theta i_{\nu_1}\cdots i_{\nu_q}\pi + \sum_{s=1}^q i_{\nu_1}\cdots i_{[\nu_s,\theta]}\cdots i_{\nu_q}\pi.$$

This last equation is easily derived by commuting L_θ backward past $i_{\nu_1}\cdots i_{\nu_q}$. Now the integral of the first term over Ω_t can be computed using Theorem 1 with $\psi = 1$ and $V = \theta$. One gets

$$\int_{\Omega_t}L_\theta\omega = \int_{\partial\Omega_t}(\theta\cdot\nu)\,\partial\omega - \int_{\Omega_t}p(\theta\cdot\mu)\omega. \tag{6}$$

The integral of the other terms is computed as follows:

$$\alpha_t^*(i_{\nu_1}\cdots i_{[\nu_s,\theta]}\cdots i_{\nu_q}\pi)$$
$$= \det\left(\frac{\partial\alpha_t}{\partial u_1},\ldots,\frac{\partial\alpha_t}{\partial u_p},\nu_1,\ldots,[\nu_s,\theta],\cdots\nu_q\right)du^1\cdots du^p$$
$$= \alpha_t^*((\nu_s\cdot\nabla_{\nu_s}\theta)\omega). \tag{7}$$

The last equation arises by expressing $[\nu_s,\theta]$ in the natural basis:

$$[\nu_s,\theta] = \sum_i a_{si}\frac{\partial\alpha_t}{\partial u_i} + \sum_i b_{si}\nu_i,$$

using this in the second step, and noting that

$$b_{ss} = \nu_s\cdot[\nu_s,\theta] = \nu_s\cdot\nabla_{\nu_s}\theta - \nu_s\cdot\nabla_\theta\nu_s$$
$$= \nu_s\cdot\nabla_{\nu_s}\theta \quad (\text{since } \nu_s \text{ is a unit vector field}).$$

Integrating (7) over U now gives

$$\int_{\Omega_t}(\nu_s\cdot\nabla_{\nu_s}\theta)\omega. \tag{8}$$

Thus the integral of $\operatorname{div}(\theta)$ in (5) reduces to

$$\int_R\left[\int_{\partial\Omega_t}(\theta\cdot\nu)\,\partial\omega + \int_{\Omega_t}\left(p\,\mu\cdot\theta - \sum_i\nu_i\cdot\nabla_{\nu_i}\theta\right)\omega\right]dt,$$

and this proves the theorem.

IV. THE DERIVATIVES ∇, div, d, d', AND $\nabla_\times$ OF DIRAC TENSOR DISTRIBUTIONS

In this section the various distributional derivatives of $\tau\delta_{\tilde\Omega}$ are calculated. The formulas involve a natural extension of the normal vector fields $\nu_1,\ldots,\nu_q,\nu$, and μ connected with the moving submanifold Ω. In general, if ξ is a vector field on R^{n+1} with no time components, $\xi_{n+1} = 0$ (Cartesian coordinates), then extend ξ to a vector field $\tilde\xi$ by taking the covariant components of $\tilde\xi$ to be

$$\tilde\xi_i = \xi_i,\quad i = 1,\ldots,n,$$
$$\tilde\xi_{n+1} = -V\cdot\xi.$$

The following theorem and its corollaries are the main results of the paper. It should be noted that in the special case when τ is a scalar field the various products: $\otimes$, $\wedge$, and $\cdot$ are just scalar multiplication.

Theorem 5: If τ is a smooth tensor field on R^{n+1}, then

$$\nabla(\tau\delta_{\tilde\Omega}) = \left[\left(\nabla\tau - \sum_i\tilde\nu_i\otimes\nabla_{\nu_i}\tau\right) + p\tilde\mu\otimes\tau\right]\delta_{\tilde\Omega}$$
$$-(\tilde\nu\otimes\tau)\delta_{\partial\tilde\Omega} - \sum_i(\tilde\nu_i\otimes\tau)\cdot\nabla_{\nu_i}(\cdot)\delta_{\tilde\Omega}, \tag{9}$$

$$\operatorname{div}(\tau\delta_{\tilde\Omega}) = \left[\left(\operatorname{div}(\tau) - \sum_i\tilde\nu_i\cdot\nabla_{\nu_i}\tau\right) + p\tilde\mu\cdot\tau\right]\delta_{\tilde\Omega}$$
$$-(\tilde\nu\cdot\tau)\delta_{\partial\tilde\Omega} - \sum_i(\tilde\nu_i\cdot\tau)\cdot\nabla_{\nu_i}(\cdot)\delta_{\tilde\Omega}. \tag{10}$$

If in addition τ is a differential form, then

$$d(\tau\delta_{\tilde\Omega}) = \left[\left(d\tau - \sum_i\tilde\nu_i\wedge\nabla_{\nu_i}\tau\right) + p\tilde\mu\wedge\tau\right]\delta_{\tilde\Omega}$$
$$-(\tilde\nu\wedge\tau)\delta_{\partial\tilde\Omega} - \sum_i(\tilde\nu_i\wedge\tau)\cdot\nabla_{\nu_i}(\cdot)\delta_{\tilde\Omega}, \tag{11}$$

and the exterior codifferential d' is equal to $-$div on such currents.

Proof: Suppose that the rank of τ is k. To derive Eq. (9), let θ be a rank-$(k+1)$ tensor field with compact support. Then

$$\langle\nabla(\tau\delta_{\tilde\Omega})|\theta\rangle = -\langle\tau\delta_{\tilde\Omega}|\operatorname{div}(\theta)\rangle$$
$$= -\langle\delta_{\tilde\Omega}|\tau\cdot\operatorname{div}(\theta)\rangle$$
$$= -\langle\delta_{\tilde\Omega}|\operatorname{div}(\theta\cdot\tau) - (\nabla\tau)\cdot\theta\rangle$$
$$= -\langle\delta_{\tilde\Omega}|\operatorname{div}(\theta\cdot\tau)\rangle + \langle(\nabla\tau)\delta_{\tilde\Omega}|\theta\rangle.$$

The first term is computed using Theorems 3 and 4 as follows (for notational convenience the $(n+1)$th contravariant component of $\theta\cdot\tau$ is denoted by $(\theta\cdot\tau)^0$):

$$-\langle\delta_{\tilde\Omega}|\operatorname{div}(\theta\cdot\tau)\rangle = -\left\langle\delta_{\tilde\Omega}\,\middle|\,\operatorname{div}\overrightarrow{(\theta\cdot\tau)} + \frac{\partial}{\partial t}(\theta\cdot\tau)^0\right\rangle$$
$$= \langle\vec\nabla\delta_{\tilde\Omega}|\overrightarrow{\theta\cdot\tau}\rangle + \left\langle\frac{\partial}{\partial t}\delta_{\tilde\Omega}\,\middle|\,(\theta\cdot\tau)^0\right\rangle$$
$$= \langle\delta_{\partial\tilde\Omega}| -\nu\cdot\overrightarrow{(\theta\cdot\tau)} + N(\theta\cdot\tau)^0\rangle$$
$$+\langle\delta_{\tilde\Omega}|\,p\,\mu\cdot\overrightarrow{(\theta\cdot\tau)} - pM(\theta\cdot\tau)^0\rangle$$
$$-\sum_i\langle\delta_{\tilde\Omega}|\nu_i\cdot\nabla_{\nu_i}\overrightarrow{(\theta\cdot\tau)} - N_i\nabla_{\nu_i}((\theta\cdot\tau)^0)\rangle.$$

Several tensor product identities can now be used to put the above expressions in the form stated in Eq. (9). For example,

$$\nu\cdot\overrightarrow{(\theta\cdot\tau)} - N(\theta\cdot\tau)^0 = \tilde\nu\cdot(\theta\cdot\tau) = (\tilde\nu\otimes\tau)\cdot\theta$$

and

$$\nu\cdot\nabla_\nu\overrightarrow{(\theta\cdot\tau)} - N\nabla_\nu((\theta\cdot\tau)^0) = \tilde\nu\cdot\nabla_\nu(\theta\cdot\tau)$$
$$= (\tilde\nu\otimes\nabla_\nu\tau)\cdot\theta + (\tilde\nu\otimes\tau)\cdot\nabla_\nu\theta.$$

Next, to derive Eq. (10) for the divergence operator, suppose that θ is a rank-$(k-1)$ tensor field with compact support. Then

$$\langle \operatorname{div}(\tau\delta_{\tilde\Omega})|\theta\rangle = -\langle \tau\delta_{\tilde\Omega}|\nabla\theta\rangle$$
$$= -\langle \delta_{\tilde\Omega}|\tau\cdot\nabla\theta\rangle$$
$$= \langle \delta_{\tilde\Omega}|\operatorname{div}(\tau)\cdot\theta - \operatorname{div}(\tau\cdot\theta)\rangle$$
$$= \langle \operatorname{div}(\tau)\delta_{\tilde\Omega}|\theta\rangle + \langle \nabla\delta_{\tilde\Omega}|\tau\cdot\theta\rangle .$$

But, calculating $\nabla\delta_{\tilde\Omega}$ from the result already proved [Eq. (9) with $\tau = 1$], one gets that the second term in the last equation is

$$\langle \delta_{\tilde\Omega}|\, p\,\tilde\mu\cdot(\tau\cdot\theta)\rangle - \langle \partial\delta_{\tilde\Omega}|\tilde\nu\cdot(\tau\cdot\theta)\rangle$$
$$-\sum_i \langle \delta_{\tilde\Omega}|\tilde\nu_i\cdot\nabla_{\nu_i}(\tau\cdot\theta)\rangle,$$

and these terms can be expressed in suitable form by using the identities:

$$\tilde\nu\cdot(\tau\cdot\theta) = (\tilde\nu\cdot\tau)\cdot\theta,$$
$$\tilde\nu\cdot\nabla_\nu(\tau\cdot\theta) = (\tilde\nu\cdot\tau)\cdot\nabla_\nu\theta + (\tilde\nu\cdot\nabla_\nu\tau)\cdot\theta .$$

Finally, if one assumes that τ is a differential form, then Eq. (11) for the exterior derivative follows easily from Eq. (9) for the absolute differential. The reason for this is that $d' = -\operatorname{div}$ on the differential forms. Thus, if θ is a $(k+1)$-form with compact support, then

$$\langle d(\tau\delta_{\tilde\Omega})|\theta\rangle = \langle \tau\delta_{\tilde\Omega}|d'\theta\rangle$$
$$= -\langle \tau\delta_{\tilde\Omega}|\operatorname{div}(\theta)\rangle = \langle \nabla(\tau\delta_{\tilde\Omega})|\theta\rangle .$$

Substituting the expression for $\nabla(\tau\delta_{\tilde\Omega})$ from Eq. (9) into this last equation, one arrives at the desired results after applying the following identities (some of which require that the connection be flat):

$$(\nabla\tau)\cdot\theta = (d\tau)\cdot\theta,$$
$$(\tilde\nu\otimes\tau)\cdot\theta = (\tilde\nu\wedge\tau)\cdot\theta,$$
$$(\tilde\nu\otimes\nabla_\nu\tau)\cdot\theta = (\tilde\nu\wedge\nabla_\nu\tau)\cdot\theta,$$
$$(\tilde\nu\otimes\tau)\cdot\nabla_\nu(\theta) = (\tilde\nu\wedge\tau)\cdot\nabla_\nu(\theta).$$

One should also note that $\nabla_\nu\theta$ is antisymmetric.

The last assertion about the operator d' is easy to see:

$$\langle d'(\tau\delta_{\tilde\Omega})|\theta\rangle = \langle \tau\delta_{\tilde\Omega}|d\theta\rangle$$
$$= \langle \delta_{\tilde\Omega}|\tau\cdot d\theta\rangle = \langle \delta_{\tilde\Omega}|\tau\cdot\nabla\theta\rangle$$
$$= \langle \tau\delta_{\tilde\Omega}|\nabla\theta\rangle = -\langle \operatorname{div}(\tau\delta_{\tilde\Omega})|\theta\rangle .$$

Corollary 1: The covariant derivative along a vector field X on R^{n+1} is given by

$$\nabla_X(\tau\delta_{\tilde\Omega}) = \left(\left[\nabla_X\tau - \sum_i \tilde\nu_i\cdot\nabla_{\nu_i}(X\otimes\tau)\right] + (p\tilde\mu\cdot X)\tau\right)\delta_{\tilde\Omega}$$
$$-(\tilde\nu\cdot X)\tau\delta_{\partial\tilde\Omega} - \sum_i(\tilde\nu_i\cdot X)\tau\cdot\nabla_{\nu_i}(\cdot)\delta_{\tilde\Omega}.$$

Proof: The proof follows from Eq. (9) and some tensor identities.

As special cases of the corollary one can take $\tau = 1$ and X a constant unit vector field either (1) in the time direction to get the result in Theorem 3 or (2) in the jth spatial direction to get the jth component of the vector expression in Theorem 4.

Another corollary to the last theorem is what amounts to a special case of it. Suppose that Ω had dimension $n-1$ and that ν_1 is a normal vector field along Ω chosen as mentioned in Sec. II. Suppose that τ is a rank m tensor field on R^{n+1} with components $\tau_{i_1\cdots i_m}$ that are smooth functions on $R^{n+1}/\tilde\Omega$. Assume that the limits

$$(\tau_{i_1\cdots i_m})_\pm(x,t) = \lim_{\epsilon\to 0}\tau_{i_1\cdots i_m}(x\pm\epsilon\nu_1(x),t)$$

exist for each t and each point x on Ω_t, and let $[\tau] = \tau_+ - \tau_-$ be the jump in τ across $\tilde\Omega$. Furthermore, let $\{\tau\}$ denote the distribution determined by τ and $\nabla\tau$, $\operatorname{div}(\tau)$, $d\tau$, and $\nabla_X\tau$ denote the functions obtained by differentiating τ where it is smooth (off $\tilde\Omega$) and assigning arbitrary values on $\tilde\Omega$. Then one gets the following:

Corollary 2: With the proper choice of content form π on R^n, the distributional derivatives of a tensor field τ which is smooth except across a moving hypersurface $\tilde\Omega$ are[10]

$$\nabla\{\tau\} = \{\nabla\tau\} + \tilde\nu_1\otimes[\tau]\delta_{\tilde\Omega}$$
$$\operatorname{div}\{\tau\} = \{\operatorname{div}(\tau)\} + \tilde\nu_1\cdot[\tau]\delta_{\tilde\Omega}$$
$$\nabla_X\{\tau\} = \{\nabla_X\tau\} + (\tilde\nu_1\cdot X)[\tau]\delta_{\tilde\Omega}.$$

Furthermore, if τ is a differential form then

$$d\{\tau\} = \{d\tau\} + \tilde\nu_1\wedge[\tau]\delta_{\tilde\Omega}$$
$$d'\{\tau\} = \{d'\tau\} - \tilde\nu_1\cdot[\tau]\delta_{\tilde\Omega}.$$

Proof: I will assume that the hypersurfaces Ω_t are reasonable ones, namely that, for each t, R^n is the union of two n-dimensional submanifolds $M_\pm(t)$ with common boundary which contains Ω_t. The labeling can be done so that ν_1 points into the region $M_+(t)$. Now π is the content form for $M_\pm(t)$, and I will assume that it is chosen so that when $\partial M_\pm(t)$ is coherently oriented with $M_\pm(t)$ the outward normal $\nu_\pm$ to $M_\pm(t)$ is such that $\nu_+ = -\nu_1$ and $\nu_- = \nu_1$. Next let $\tilde M_\pm$ be the tube swept out in R^{n+1} by $M_\pm(t)$. One can construct two smooth tensor fields $T_\pm$ on R^{n+1} so that $T_\pm = \tau$ on $M_\pm/\tilde\Omega$ and $T_\pm = \tau_\pm$ on $\tilde\Omega$ (cf. the schematic Fig. 3). From this, one gets that

$$\{\tau\} = T_+\delta_{\tilde M_+} + T_-\delta_{\tilde M_-}$$

and (approximately)

$$\delta_{\partial\tilde M_+} = \delta_{\partial\tilde M_-} \cong \delta_{\tilde\Omega}.$$

Applying Theorem 5 to $T_\pm\delta_{\tilde M_\pm}$ and noting that in each case $\mu^\pm = 0$ and $\tilde\nu_i^\pm = 0$ (by convention) one arrives at

$$\nabla\{\tau\} = \nabla T_+\delta_{\tilde M_+} + \nabla T_-\delta_{\tilde M_-}$$
$$-\tilde\nu_+\otimes T_+\delta_{\partial\tilde M_+} - \tilde\nu_-\otimes T_-\delta_{\partial\tilde M_-}$$
$$= \{\nabla\tau\} + \nu_1\otimes[\tau]\delta_{\tilde\Omega}.$$

The assertions about the other differential operators are thus seen to follow in a similar fashion.

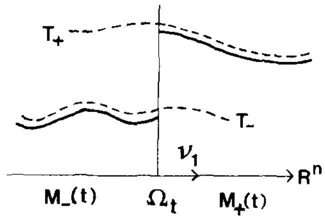

FIG. 3. Schematic extensions (dotted lines) of a tensor field (solid line) with jump discontinuity across the hypersurface Ω_t.

V. CONCLUSION

In conclusion I would like to include a few comments concerning the derived expressions. These are directed toward questions as to the form and geometrical significance of these expressions.

If D stands for one of the differential operators ∇, ∇_X, div, d, d', then the results of the last section gives that $D(\tau\delta_{\tilde{\Omega}})$ may be expressed in the form

$$D(\tau\delta_{\tilde{\Omega}}) = A\delta_{\partial\tilde{\Omega}} + B\delta_{\tilde{\Omega}} + \sum_i C_i\cdot\nabla_{\nu_i}(\cdot)\delta_{\tilde{\Omega}}. \tag{12}$$

There are other forms in which this result may be expressed, but the advantage of the form above is that it is a disjoint decomposition in the sense that if

$$D(\tau\delta_{\tilde{\Omega}}) = A'\delta_{\partial\tilde{\Omega}} + B'\delta_{\tilde{\Omega}} + \sum_i C'_i\cdot\nabla_{\nu_i}(\cdot)\delta_{\tilde{\Omega}},$$

then $A = A'$ on $\partial\Omega$ and $B = B'$, $C_1 = C'_1, ..., C_q = C'_q$ on $\tilde{\Omega}$. Thus, in particular, the equation $D(\tau\delta_{\tilde{\Omega}}) = 0$ allows one to equate the coefficients in (12) to zero.

To comment further on the nature of expression (12), I will only consider the operator $D = \nabla_X$ which has the familiar geometric interpretation of being the partial derivative in the X direction (on classical fields). Then since

$$\langle\nabla_X(\delta_{\tilde{\Omega}})|\psi\rangle = -\langle\delta_{\tilde{\Omega}}|\mathrm{div}(\psi X)\rangle,$$

one could write that

$$\nabla_X(\delta_{\tilde{\Omega}}) = -\mathrm{div}[(\cdot)X]\delta_{\tilde{\Omega}}.$$

However, this fails to capture the underlying geometric significance of this derivative of the delta function. For the sake of example, consider the cases of a solid body $\widetilde{M}$, a surface $\widetilde{S}$, a curve $\widetilde{C}$, and a point $\tilde{a}$ all moving in R^3 as shown in Figs. 1 and 2. The formulas from the last section give in these cases:

$$\nabla_X(\delta_{\tilde{M}}) = -(\tilde{\nu}\cdot X)\delta_{\partial\tilde{M}}, \tag{13}$$

$$\nabla_X(\delta_{\tilde{S}}) = -(\tilde{\nu}\cdot X)\delta_{\partial\tilde{S}} + 2H(\tilde{\nu}_1\cdot X)\delta_{\tilde{S}} - (\tilde{\nu}_1\cdot X)\nabla_{\nu_1}(\cdot)\delta_{\tilde{S}}, \tag{14}$$

$$\nabla_X(\delta_{\tilde{C}}) = -(\tilde{\nu}\cdot X)\delta_{\partial\tilde{C}} + \kappa(\tilde{\nu}_1\cdot X)\delta_{\tilde{C}} - \sum_{i=1}^{2}(\tilde{\nu}_i\cdot X)\nabla_{\nu_i}(\cdot)\delta_{\tilde{C}}, \tag{15}$$

$$\nabla_X(\delta_{\tilde{a}}) = -\sum_{i=1}^{3}(\tilde{\nu}_i\cdot X)\nabla_{\nu_i}(\cdot)\delta_{\tilde{a}}. \tag{16}$$

Here the freedom in the choice of the normal vector fields ν_i has been exploited to obtain simpler formulas. For M there is no choice to make. For S the normal field ν_1 is determined up to a sign but the mean curvature normal $\mu = H\nu_1$, where H is the mean curvature, is the same regardless of the choice of ν_1. For the curve C with unit tangent vector l one can always choose ν_1 and ν_2 so that l, ν_1, ν_2 is the distinguished Frenet frame along C. Then ν_1 is the normal, ν_2 the binormal, and $\mu = \kappa\nu_1$, where κ is the curvature function for C. In the case of a moving point $\tilde{a}$ one can choose ν_1, ν_2, and ν_3 to be any constant unit vector fields on R^3 (which are mutually orthogonal and positively oriented) to obtain formula (16).

A particularly nice feature of these formulas is that the normal derivatives in the direction $X = -\nu$ yield Dirac delta functions (a generalization of the well-known fact that the derivative of Heaviside's function is Dirac's delta function):

$$\nabla_X(\delta_{\tilde{M}}) = \delta_{\partial\tilde{M}},$$

$$\nabla_X(\delta_{\tilde{S}}) = \delta_{\partial\tilde{S}},$$

$$\nabla_X(\delta_{\tilde{C}}) = \delta_{\partial\tilde{C}}.$$

Thus one sees how the geometry of the submanifold, except in the case of a point (which has no geometry), influences the form of the derivative, and this to a greater extent the greater the dimension of the submanifold.

[1]David E. Betounes, J. Math. Phys. **23**, 2304–11 (1982).

[2]Robert C. Costen, J. Math. Phys. **22**, 1377–85 (1981).

[3]In the notation established later in the paper $\rho\delta_{\tilde{C}}$ and $J\delta_{\tilde{C}}$ represent charge and current distributions along a moving curve C. Also $\rho\delta_{\tilde{S}}$ represents a moving charged surface and $J\delta_{\tilde{S}}$ a moving current sheet.

[4]R. Estrada and R. P. Kanwal, J. Inst. Math. Appl. **26**, 39–63 (1980).

[5]David E. Betounes, "Applications of nonclassical field theory I: Electromagnetic diffusion" (submitted for publication).

[6]Some standard references for differential geometry and distribution theory are: (a) S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry* (Wiley, New York, 1963 and 1969), Vols. I and II; (b) Yvonne Choquet-Bruhat, Cécile deWitt-Morrette, and Margaret Dillard-Bleick, *Analysis, Manifolds, and Physics* (North-Holland, Amsterdam, 1977); (c) Walter Thirring, *A Course in Mathematical Physics* (Springer-Verlag, New York, 1978), Vol. I; (d) Francois Trèves, *Topological Vector Spaces, Distributions, and Kernels* (Academic, New York, 1967).

[7]See Ref. 6(b) p. 208.

[8]The definition of $\tau\delta_{\tilde{\Omega}}$ can be motivated by the following consideration. If $\tilde{a} = \{a(t)|t\in R\}$ is the world line of a moving point in R^3 and if ρ is a constant, then the definition gives

$$\langle\rho\delta_{\tilde{a}}|\psi\rangle = \int_R \rho\psi(a(t),t)\,dt$$

and $\rho\delta_{\tilde{a}}$ represents a particle which charge ρ moving in R^3. This should be contrasted with the Dirac delta function for a point $x = (\mathbf{x}_0, t_0)$ in spacetime. Here the definition is

$$\langle\rho\delta_x|\psi\rangle = \rho\psi(\mathbf{x}_0, t_0)$$

and so $\rho\delta_x$ represents a particle with charge ρ which only exists at the instant t_0 in time and the point $\mathbf{x}_0$ in space.

[9]David E. Betounes, Am. J. Phys. **51**, 554–560 (1983).

[10]These formulas generalize the ones given in Ref. 6(b), p. 369.

Realization of Gaussian random fields

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The representation of stationary Gaussian processes in terms of filtered Gaussian white noise is studied. Known results are extended from the finite-dimensional case to the dimension-free case; hence, in particular, to Gaussian random fields. In particular, the following result is proved for usual Gaussian processes: Physical realizability is equivalent to realizability.

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INTRODUCTION

In the present study, "process" means "centered and stationary Gaussian process."

0.1. Markov realization

The operator of time derivation is denoted D. If X and K are two locally convex Hausdorff spaces (l.c.H.s.), $L(X, K)$ denotes the set of all linear and continuous maps: $X \to K$. In particular, End $X = L(X, X)$ denotes the set of all endomorphisms of X. The transposition $A \to A^T$ maps $L(X, K)$ in $L(K', X')$. The usual theory of Markov realization[1] is first recalled. A process (g_t) on the line with values in $\mathbb{R}^p$ is called realized in dimension n if (g_t) is a linear observation of a process $\xi = (\xi_t)$ with values in $\mathbb{R}^n$, ξ satisfying the following two conditions (a) and (b):

(a) $\exists A^T \in \text{End } \mathbb{R}^n$ such that

$$D\xi - A^T \xi = N, \tag{0.1}$$

where N denotes a Gaussian white noise.

(b) The stochastic process ξ is physically realized by filtering N, i.e., there exists a causal filter $h^T \in L^2(\mathbb{R}^+, \text{End } \mathbb{R}^n)$ such that $\xi = h^T * N$.

If the covariance of ξ_0 is invertible, this implies $h^T(t) = \exp_+(tA^T)$ and A^T asymptotically stable, i.e., each eigenvalue of A^T has a negative real part. Therefore,

$$\exists B^T \in L(\mathbb{R}^n, \mathbb{R}^p), \quad (g_t) = B^T(\xi_t), \tag{0.2}$$

and the spectral densities S_g of the realizable processes can be characterized: S_g is rational in the scalar case $p = 1$, and of rational type (4.1) for $p > 1$. The realization of processes with a given spectral density of this type has been studied extensively.

Realizable processes are important, since they have extended the domain of applicability of Kolmogoroff's and Ito's techniques from differential systems driven by Gaussian white noises to differential systems driven by Gaussian realizable processes (g_t) and with independent white noises dW/dt. The idea is to replace a stochastic differential equation

$$d\eta_t = b(t, \eta_t, g_t)\, dt + a(t, \eta_t, g_t)\, dW_t \tag{0.3}$$

by the stochastic equation of Ito type satisfied by the process (ξ_t, η_t), with values in $\mathbb{R}^n \oplus \mathbb{R}^p$:

$$d\begin{pmatrix}\xi_t \\ \eta_t\end{pmatrix} = \begin{pmatrix}A^T\xi \\ b(t, \eta_t, B^T\xi_t)\end{pmatrix} dt + \begin{pmatrix}N_t\, dt \\ a(t, \eta_t, B^T\xi_t)\, dW_t\end{pmatrix}.$$

Physically, this means that for differential equations with colored input arising in nonlinear filtering, stochastic control, random mechanics..., an auxiliary differential equation (0.1) and an appropriate observation map B^T can be built up in order that the colored input (g_t) is well modelized by $(B^T\xi_t)$.

0.2. Problems concerning Markov realizations

This leads to several problems.

A. Problem of stability and of approximate realization

Practically, the process g arising in (0.3) is an approximation of a given physically realizable process g'. Is it possible to realize g'? Can the realization of g be considered as an approximate realization of g'?

N.B: In usual realization methods, the probability space used for the construction of the process (ξ_t, η_t) depends on S_g. Hence, a probabilistic study concerning an infinite set of spectral densities is difficult using this approach.

B. Problems concerning driving signals generated by distributed parameter systems

Sometimes the driving signal (g_t) is a linear observation of a distributed parameter system; and the equation governing the state (ξ_t) of this system is of the type (0.1), with $\mathbb{R}^n$ replaced by an appropriate functional space. What kind of observed signals are obtained in this case? Since computers work only with finite sets of numbers, how can the observed signal $(B^T\xi_t)$ be approximated by a signal possessing a finite-dimensional realization?

C. Problems concerning driving signals, generated by observation of random fields

Often, the driving signal (g_t) is an observation of a random Gaussian field $(c_{t,x})$, x belonging to some open subset I of $\mathbb{R}^d$; c is statistically characterized by an experimental correlation function. But, viewing c as a vector-valued process (C_t) with values in $\mathscr{D}'(I)$, (C_t) is, in general, not governed by an equation of the type (0.1). In order to construct realizations and approximate realizations for (g_t), is it possible to realize (C_t)? The problem of realization of random fields is also of interest in connection with partial differential equations (p.d.e) with random coefficients. Consider, for example, a random field $(u_{t,x})$ on $\mathbb{R}\times I$, a solution of the heat equation

$$D_t u_{t,x} = c_{t,x}\, \Delta u_{t,x} \quad + \text{boundary conditions.} \tag{0.4}$$

The fields u and c are replaced by the corresponding vectorial processes (U_t) and (C_t). If (C_t) is a linear observation of some auxiliary "Markov" process ξ_t generated by a Gaussian white noise, then $(\xi_t; U_t)$ is the solution of a vectorial Ito's equation; hence, Kolmogoroff's and Ito's constructive techniques can be applied.

For these reasons, an extension for arbitrary n and p of the usual realization theory is needed. In the formulation given below, only stationary-centered Gaussian processes are considered, even if other applications are possible. In the present case, techniques of functional analysis seem to be more appropriate than usual techniques of probability theory, since singular linear transforms of Gaussian measures are used. Hence, triplets and cylindrical processes (c.p.) are used: This means that, for any fixed time t, the random variable (r.v.) ξ_t is identified with the corresponding linear process (l.p.) $x\to\langle\xi_t, x\rangle$. This l.p. is defined on some space in duality with the space where the probability distribution of ξ_t lives. For these reasons, transpositions $A\to A^T$, $B\to B^T$... are frequently used.

Section 1 gives the notations and introduces the concept of c.p. (g_t) physically realized by filtering a given Gaussian white noise. The connection with the usual concept of realizability is:

If the values of (g_t) are linear processes on a finite-dimensional vector space Y, up to an isonomy, (g_t) is physically realizable for filtering *some* Gaussian white noise iff the stochastic process with values in Y' defined by (g_t) is physically realizable, in the usual meaning.

Section 2 gives a dimension-free extension of Doob's result characterizing the $A^T\in\mathrm{End}\ \mathbb{R}^n$ such that 0.1(a) and 0.1(b) are true for some process (ξ_t). Evidently, an additional hypothesis is needed for the infinitesimal generator, since "unbounded operators" are introduced, and since the exponential of such operators are not defined, in general. The direct part of the characterization is.

0.3. Direct assertion: Necessary conditions for the construction of ξ

Let X be the completion of a barreled space X_i for the scalar product $\langle Cx, x\rangle$, where C is symmetric, positive, and injective $\in L(X_i, X_i')$. Let $t\to\exp tF$ be a semigroup of operators $\in L(X_i) = L(X_i, X_i)$. Let (ξ_t) be a continuous c.p. on the line, with values l.p.'s on X_i such that

(i) $\forall t$, the covariance of ξ_t is C,
(ii) $D\xi - F^T\xi$ is a Gaussian white noise N,
(iii) ξ is physically realizable by filtering N.

Then, necessarily, the semigroup $(\exp tF)$ defines by continuous extension a semigroup of contractions $t\to\exp tA$ in X, satisfying the following condition:

$$\forall x\in X, \quad \|(\exp tA)x\|_X\to 0 \quad \text{if } t\to\infty. \tag{C}$$

The assertion 2.3 shows that, conversely, for any Hilbertian data of this type, a corresponding continuous c.p. (ξ_t) satisfying (i), (iii), and

(ii') $D\xi - A^T\xi$ is a Gaussian white noise N

can be constructed. In the particular case where $\dim X = n$ is finite, this gives Doob's characterization of A: A is asymptotically stable, i.e., all eigenvalues of A satisfy $\mathrm{Re}\,\lambda < 0$. In Sec. 2.5, the spectral density of any linear observation $(g_t) = (B^T\xi_t)$ of the c.p. (ξ_t) is computed; since the usual expression of this density, in the finite-dimensional case, has, in general, no meaning in the dimension-free case, another expression is proposed [see (2.8)]. We also prove that the realized c.p. (g_t) is necessarily physically realized by filtering N; but the converse property is not evident. For example, in the one-dimensional case, it was not known whether scalar processes with spectral densities of the type $\exp(-|\omega|)$, or $(1+\omega^2)^\alpha$ with $\alpha < -\frac{1}{2}\cdots$, are realizable. The results of Secs. 1–3 are combined to prove the following theorem:

0.4. Theorem of simultaneous realization

For any Gaussian white noise N, a c.p. (ξ), as previously defined, can be constructed such that all c.p. physically realized by filtering N are realized by observing ξ.

Since no restriction on dimension is assumed, this theorem gives a solution to the problems B and C (Sec. 0.2). As an illustration, explicit realizations are given in Sec. 4 for Gaussian random fields on $\mathbb{R}\times\mathbb{R}^d$ with spectral measure

$$(1+\omega^2+|\xi|^2)^\alpha \tag{0.5}$$

with $\alpha < -(d+1)/2$ and $\xi = (\xi_1\cdots\xi_d)$, $d = 0, 1\ldots$.

Since all physically realizable processes generated by a given white noise N are realized simultaneously, the last theorem gives a method of resolution for the problem A. These results were announced in *Compte-Rendus* notes[2] and Ref. 3.

1. PHYSICAL REALIZATION BY FILTERING A GIVEN NOISE

If X and K are two real l.c.H.s., the space $L(X, K)$ is endowed with the topology of uniform convergence on all finite subsets of X. If, for example, K is the Hilbert space $L^2(\Omega)$ of all second-order random variables (r.v.), $L(X, L^2(\Omega))$ is the space of all continuous second-order linear processes on X. Below we work only with centered $R\in L(X, L^2(\Omega))$, i.e., such that $E(\langle R, x\rangle) = 0$ for all $x\in X$. Such processes will simply be called "linear processes."

1.1. Covariance and stochastic Hilbert space

For $R\in L(X, L^2(\Omega))$, the covariance is the linear operator $C: X\to X'$ such that

$$\forall x, y\in X, \quad \langle Cx, y\rangle_{X'\times X} = E(\langle R, x\rangle\langle R, y\rangle). \tag{1.1}$$

Then $\ker C = \ker R$. The canonical decomposition of the linear map R is $X\to X/\ker C\to \mathrm{Im}\,R\hookrightarrow L^2(\Omega)$. Introducing the closure of $\mathrm{Im}\,R$ in $L^2(\Omega)$ and the completion X_c of $X/$

ker C for the scalar product $(\dot{x};\dot{y})\mapsto\langle Cx, y\rangle$, the following factorization of R is constructed:

$$X \xrightarrow{j_c} X_c \xrightarrow{\simeq} \overline{\operatorname{Im} R} \hookrightarrow L^2(\Omega), \tag{1.2}$$

where the central map is bijective and isometric. For this reason, X_c is called th stochastic Hilbert space of R, or of the positive quadratic form $\langle Cx, x\rangle$ on X.

1.2. Cylindrical processes

A cylindrical process (resp. a continuous c.p.) on the line, with linear process values on some l.c.H.s. X is a map (resp. a continuous map) (ξ_t): $\mathbb{R}\to L(X, L^2(\Omega))$. The covariance of (ξ_t) is the map $C_\xi: \mathbb{R}\times\mathbb{R}\to L$ (X weak, X' weak) defined in the following way for arbitrary t, $u\in\mathbb{R}$, x and $y\in X$:

$$\langle C_\xi(t,u)x, y\rangle = E(\langle\xi_t, y\rangle\langle\xi_u, x\rangle). \tag{1.3}$$

Note that a c.p. is continuous iff the covariance is continuous.

A cylindrical process (ξ_t) is called stationary if $\forall h$ real (ξ_t) is isonomic with the translated cylindrical process $(\xi_{t+h})_t$; then

$$C_\xi(t,u) = C_\xi(t-u); \quad C_\xi(-t) = C_\xi(t)^T \quad \text{and } \forall t$$
the covariance of the linear process ξ_t is $C_\xi(0)$. (1.4)

1.3. Generalized cylindrical processes

A generalized c.p. (ξ_φ) on the line, with linear processes values on X is a linear and continuous map $\mathscr{D}(\mathbb{R})\to L(X, L^2(\Omega))$.

It is convenient to write informally $\xi_\varphi = \int \xi_t\varphi(t)\,dt$, even for a generalized c.p., which is not defined in the following way by a continuous c.p. (ξ_t):

$\forall\varphi\in\mathscr{D}(\mathbb{R}) \quad \forall x\in X$,

$$\langle\xi_\varphi, x\rangle = \int \varphi(t)\langle\xi_t, x\rangle\,dt. \tag{1.5}$$

In the same way, the covariance $C_\xi: \mathscr{D}(\mathbb{R})^2\to L$ (X weak, X' weak) is defined mathematically in the following way, for arbitrary φ, $\psi\in\mathscr{D}(\mathbb{R})$, x and $y\in X$,

$$\langle C_\xi(\varphi,\psi)x, y\rangle = E(\langle\xi_\varphi, y\rangle\langle\xi_\psi, x\rangle). \tag{1.6}$$

But it is convenient to write informally

$$C_\xi(\varphi,\psi) = \iint C_\xi(t,u)\varphi(t)\psi(u)\,dt\,du, \tag{1.7}$$

and also $C(t,u) = C(t-u)$ if (ξ_ψ) is stationary.

1.4. Gaussian white noise

Let X be an l.c.H.s.; let X_Q be the stochastic Hilbert space of $\langle Qx, x\rangle$, where Q is positive and symmetric $\in L(X, X')$. The canonical injection of $\mathscr{D}(\mathbb{R})$ in $L^2(\mathbb{R})$ is denoted j. Identifying isometrically $L^2(\mathbb{R}, X_Q)$ with a space of Gaussian r.v., the corresponding white noise N is the generalized c.p.: $\mathscr{D}(\mathbb{R})\otimes X\to L^2(\mathbb{R}, X_Q)$ defined by the composition of $j\otimes j_Q$ with the canonical injection $L^2(\mathbb{R})\otimes X_Q \to L^2(\mathbb{R}, X_Q)$. A computation gives the covariance of N: $C_N = \delta_0(t-s)Q$. We write informally $N_\varphi = \int N_t\varphi(t)\,dt$. Working only with stationary-centered Gaussian cylindrical processes, with continuous stationary-centered Gaussian c.p., and with stationary-centered Gaussian generalized c.p., notations are simplified to "c.p.," "continuous c.p.," and "generalized c.p.."

1.5. Extension of the usual concept of linear filter

In order to explain the connection between familiar linear filters and the definition of linear filters given below, we first consider the particular case where X is a finite-dimensional Euclidean space. A linear filter adapted to N is usually defined as an element

$$h^T\in L^2(\mathbb{R}, L(X', Y')), \tag{1.8}$$

where Y' is the dual of some Euclidean space Y. The filtered process h^T*N takes values in Y' and is given by

$$(h^T*N)_t = \int_{-\infty}^{+\infty} h(t-u)^T N_u\,du. \tag{1.9}$$

This process is defined by the following c.p. on the line with linear process values on Y:

$$y\mapsto\langle(h^T*N)_T, y\rangle = \left\langle\int_{-\infty}^{+\infty} h(t-u)^T N_u\,du, y\right\rangle.$$

Hence using the transpose $(h(t)^T)^T = h(t)\in L(Y, X)$ of $h(t)^T$,

$$\langle(h^T*N)_t, y\rangle = \langle N_u, h(t-u)y\rangle. \tag{1.10}$$

The rhs denotes the Gaussian r.v. associated by N with the element $u\to h(t-u)y$ of the stochastic Hilbert space of N.

The definitions (1.9) and (1.10) are not convenient in the infinite-dimensional case for the following reasons:

- The space $L(X', Y')$ has no canonical Hilbertian structure.
- (1.8) and (1.9) are not well adapted to the covariance of N.

Therefore, (1.10) is chosen in order to define linear filter if dim X and dim Y are arbitrary.

1.6. Linear filters

If Y denotes a l.c.H.s, an element $h\in L(Y, L^2(\mathbb{R}, X_Q))$ is called a filter defined on Y adapted to N. The image of $y\in Y$ by this map is denoted $t\mapsto h(t)y$. Filtering N with this filter gives the c.p. $g = h^T*N$ such that

$$\forall t, \quad \forall y\in Y, \quad \langle g_t, y\rangle = N_u(h(t-u)y). \tag{1.11}$$

The covariance of (g_t) can be computed

$$\langle C_g(t)y, y'\rangle = \int_{u\in\mathbb{R}} \langle h(u)y, h(t+u)y'\rangle_Q\,du. \tag{1.12}$$

Hence using (1.6), (g_t) is necessarily a continuous c.p. By the Plancherel theorem, $\forall y\in Y$, the Fourier transform (FT) of $h(t)y$ belongs to $L^2(\mathbb{R}, X_Q)$ and this element is denoted $H(\omega)y$. The following convention is used for FT:

$$H(\omega)x = \int_{-\infty}^{+\infty} h(t)xe^{-it\omega}\,dt. \tag{1.13}$$

Putting $\check{h}(t)y = h(-t)y$, for y and y' fixed $\in Y$, the function $\langle C_g\,y, y'\rangle$ is the convolution, associated with the bilinear map defined by the scalar product of X_Q, of the vectorial functions hy' and $\check{h}\,y$. Hence, $\mathscr{F}\langle C_g\,y, y'\rangle\in L^1(\mathbb{R})$. Moreover for fixed t, $\langle C_g(t)y, y'\rangle$ is separately continuous with respect to y and $y' \in Y$. The spectral measure of g is defined by $S_g = (2\pi)^{-1}\mathscr{F}C_g$: This is a distribution on the line, with values in $L(X, X')$. For arbitrary $y\in Y$, $\langle S_g\, y, y\rangle$ is an integrable function on the line, and for almost all real ω,

$$\langle S_g(\omega)y, y\rangle = (\|H(\omega)y\|_Q)^2. \tag{1.14}$$

N.B.: S_g is not a measure, but a $\mathscr{G}$-cylindrical measure.[4]

1.7. Causal filter

A filter $h_+ \in L(Y, L^2(\mathbb{R}, X_Q))$ is called causal if h_+ is the product of some element $h\in L(Y, L^2(\mathbb{R}^+, X_Q))$, with the canonical injection $L^2(\mathbb{R}^+, X_Q) \to L^2(\mathbb{R}, X_Q)$; sometimes we simply write $h = h_+$. In order to connect FT and Laplace transform (LT),

$$p \mapsto \int_0^\infty (h(t)x)e^{-pt}\, dt, \quad \operatorname{Re} p \geqslant 0, \tag{1.15}$$

the FT is viewed as a function on the imaginary axis of the complex plane $p = u + i\omega$. Hence, for any causal filter $h\in L(Y, L^2(\mathbb{R}^+, X_Q))$ and $y\in Y$, Hy belongs to the Hardy class

$$H^+(X_Q) = \mathscr{F}(L^2(\mathbb{R}^+, X_Q)). \tag{1.16}$$

Any element in this Hardy class can be viewed as the boundary value of a holomorphic function on the right complex plane $\operatorname{Re} p \geqslant 0$.

1.8. Physical realizability by filtering a given white noise N

Let N be as before. A continuous c.p. (g_t) with values l.p. on some l.c.H.s. Y is called physically realized by filtering N, (resp. physically realizable by filtering N) if there exists a causal filter $h\in L(Y, L^2(\mathbb{R}^+, X_Q))$ such that $g = h * N$ (resp. such that g is isonomic with $h * N$).

2. ANALYSIS OF THE CONSTRUCTION OF (ξ_t)

2.1. Definition

First, the terminology used in the direct assertion (0.3) is detailed.

Linear maps F and $e(t) = \exp tF \in L(X_i)$ are given for all $t \geqslant 0$ such that $e(0) = \mathrm{Id}(X_i)$, $e(t)e(t') = e(t+t')$ for all t and $t' \geqslant 0$, and

$$\forall x\in X, \quad h^{-1}(e(h) - 1)x - Fx \to 0 \quad \text{in} \quad X_i \quad \text{if} \quad h \downarrow 0.$$

The generalized c.p. $D\xi$ and the c.p. $F^T\xi$ are respectively defined by $(D\xi)_\varphi = -\xi_{D\varphi}$ and $\langle F^T\xi_t, x\rangle = \langle \xi_t, Fx\rangle$ for arbitrary real t, $x\in X$ and $\varphi\in\mathscr{D}(\mathbb{R})$.

2.2. Proof of the direct assertion section 0.3

Since X_i is barreled, X_i' weak is quasi-complete; hence Ref. 5 shows that the canonical injection j' of X_i in X is weakly continuous. Transposing j', a triplet is built up: $X \hookrightarrow X = X' \hookrightarrow X_i'$ such that the identity map Id X of X induces C. The causal filter $k\in L(X_i, L^2(\mathbb{R}, X_Q))$ generating (ξ_t) is introduced:

$$\forall t, \quad \forall x\in X_i, \quad \langle \xi_t, x\rangle = N_u(k(t-u)x).$$

Hence $\forall \varphi\in\mathscr{D}(\mathbb{R})$,

$$\langle \xi_\varphi, x\rangle = N_u\left[\int_{-\infty}^{+\infty} (k(t-u)x)\varphi(t)\, dt\right],$$

$$\langle (D\xi)_\varphi, x\rangle = -\langle \xi_{D\varphi}, x\rangle = -\left[\int_{-\infty}^{+\infty} (k(t-u)x)D\varphi(t)\, dt\right].$$

Therefore, the relation $D\xi - F^T\xi = N$ is equivalent to the following equalities of distributions on $\mathbb{R}$, with values in X_Q,

$$\forall x\in X_i, \quad D(k(t)x) - k(t)(Fx) = \delta_0 \otimes (j_Q x). \tag{2.1}$$

For arbitrary $x\in X$, the distribution $(k(t)x)dt$ vanishes for $t \leqslant 0$. It is easy to show that $(k(t)x)dt$ is represented for all t by a continuous function $\mathbb{R} \to X_Q$, Frechet-derivable on $]0, +\infty[$. Hence, for arbitrary fixed t, $k(t)$ is defined $\in L(X_i, X_Q)$.

We now prove

$$\forall t \geqslant 0, \quad \forall x\in X, \quad k(t)x = e(t)x. \tag{2.2}$$

In fact, the distributions represented by the functions $k_0(t)x = j_Q(e_+(t)x)$ vanish for $t<0$, and satisfy the following differential equations on the line:

$$D(k_0(t)x) - k_0(t)(Fx) = \delta_0 \otimes (j_Q x).$$

Hence $\forall x\in X_i$, the difference $l(t)x = k(t)x - k_0(t)x$ is a continuous function $\mathbb{R} \to X_Q$, vanishing for $t \leqslant 0$, solution of

$$D(l(t)x) - l(t)(Fx) = 0.$$

The following lemma, well known for Banach spaces valued and strongly derivable functions, will be used:

Let $f(t)$ be a Frechet-derivable map defined on $I =]0, 1[$, with values in a barreled space X_i, and let g be a Frechet-derivable map on I, with values in the weak space X_i'. Then $h(t) = \langle f(t), g(t)\rangle$ is a derivable numerical function and

$$Dh = \langle Df, g\rangle + \langle f, Dg\rangle.$$

In order to prove (2.2), we prove only

$$\forall y\in X_i, \quad \forall t_1 > 0, \quad \langle l(t_1)x, j_Q y\rangle = 0. \tag{2.3}$$

The following function defined for $0 \leqslant t \leqslant t_1$,

$$h(t) = \langle j_Q(y), l(t)(e(t_1 - t)x)\rangle$$

vanishes for $t = 0$, has a vanishing derivative for $0 < t < t_1$. Hence $h(t_1) = 0$; this proves (2.3) and (2.2). Therefore, $x \to j_Q(e(t)x)$ is a causal filter; hence $\forall x\in X_i$,

$$\int_0^\infty \|j_Q(e(t)x)\|^2\, dt = \int_0^\infty \langle e(t)^T Q e(t)x, x\rangle\, dt < \infty. \tag{2.4}$$

Since $C_\xi(0) = C = \mathrm{Id}(X)$, Formula (1.16) gives

$$\forall x\in X_i, \quad \langle x, x\rangle = \int_0^\infty \langle e(u)^T Q e(u)x, x\rangle\, du. \tag{2.5}$$

Therefore

$$\begin{aligned}\langle (F + F^T)x, x\rangle &= \int_0^\infty \langle (F^T e(u)^T Q e(u) \\ &\qquad + e(u)^T Q e(u) F)x, x\rangle\, du \\ &= \int_0^\infty d\,\langle e(u)^T Q e(u)x, x\rangle \\ &= \lim_{t\to\infty} \int_0^t \cdots \\ &= -\langle Qx, x\rangle + \lim_{t\to\infty} \langle e(t)^T Q e(t)x, x\rangle.\end{aligned}$$

In view of (2.4), the last limit vanishes. Hence,

$$Q = -F - F^T \tag{2.6}$$

$$\forall x \in X_i, \quad \lim_{t\to\infty} \langle Qe(t)x, e(t)x\rangle = 0. \tag{2.7}$$

The previous lemma shows that the function $t \to \|(\exp tF)x\|^2$ is derivable; since Q is positive,

$$\left(\frac{d}{dt}\right)\|(\exp tF)x\|^2 = \langle (F + F^T)(\exp tF)x, (\exp tF)x\rangle \leqslant 0.$$

Hence $\forall t \; \|(\exp tF)x\|^2 \leqslant \|x\|^2$.

Hence $\exp tF$ defines by continuous extension a linear contraction of X denoted $\exp tA$. The semigroup property of $t \to \exp tA$ follows using a continuity argument from the semigroup property of $t \to e(t)$. For any fixed $x \in X$, the map $t \mapsto (\exp tA)x$ is the uniform limit of the sequence of continuous functions $t \mapsto (\exp tF)x_n$ if $\|x_n - x\| \to 0$. Hence $t \mapsto \exp tA$ is a continuous semigroup of contractions. Moreover, the domain of the infinitesimal generator A contains X_i and $A = F$ on X_i. Finally, $\forall x \in X_i$,

$$D\|e(t)x\|^2 = 2\langle Fe(t)x, e(t)x\rangle = -\langle Qe(t)x, e(t)x\rangle.$$

Hence by integration and using (2.5),

$$\|x\|^2 = -\lim_{t\to\infty} \int_0^t d(\|e(u)x\|^2)$$

$$= \|x\|^2 - \lim_{t\to\infty} \|e(t)x\|^2.$$

Hence $\|(\exp tA)x\| \to 0$ for $t \to +\infty$ for all x belonging to the dense subspace X_i of X. Since $\|\exp tA\| \leqslant 1$, the condition (C) (Sec. 0.3) follows. This proves the direct assertion.

2.3. Converse assertion, concerning the construction of ξ

Let $t \to \exp tA$ be a continuous semigroup of linear contractions of a real Hilbert space X, satisfying the condition (C). Endowing Dom A with the graph norm, transposing the canonical injection of Dom A in X and A, we obtain a triplet Dom $A \hookrightarrow X \hookrightarrow (\text{Dom } A)'$ and a bounded operator $A^T_{\text{ext}} : X \to (\text{Dom } A)'$ extending the transpose A^T of the linear operator A of X. Then $Q = -A - A^T_{\text{ext}} : \text{Dom } A \to (\text{Dom } A)'$ is symmetric and positive $\in L(\text{Dom } A, (\text{Dom } A)')$. Endowing (Dom A) with the norm induced by X, the map $x \to j_Q(\exp tA)x$: Dom $A \to L^2(\mathbb{R}, X_Q)$ is an isometry whose continuous extension is denoted $x \to j_Q(\exp tA)x$. Then for any Gaussian white noise N with covariance $\delta_0(t-s)Q$, the restriction ξ of $\hat{\xi} = (j_Q(\text{ext } A))*N$ to the subspace Dom A of X satisfies the three conditions:

(i) $\forall t$, the covariance of ξ_t is Id (X),

(ii) $D\xi - A^T\xi = N$, where $A^T\xi$ is defined by $\langle A^T\xi_t, x\rangle = \langle \hat{\xi}_t, Ax\rangle$,

(iii) (ξ_t) is physically realized by filtering N.

Proof: For arbitrary $x \in \text{Dom } A$,

$$\frac{d}{dt}\|(\exp tA)x\|^2 = 2\langle A(\exp A)x, (\exp tA)x\rangle$$

$$= -\langle Q(\exp tA)x, (\exp tA)x\rangle. \quad *$$

Since $t \to \|(\exp tA)x\|^2$ decreases for small t $-\langle Qx, x\rangle \leqslant 0$ for arbitrary $x \in \text{Dom } A$. Hence Q is a positive symmetric element of L (Dom A,(Dom A)'). Now, by integration of $*$ on a finite time interval,

$$\int_0^t \langle Q(\exp uA)x, (\exp uA)x\rangle\, du$$

$$= \|x\|^2 - \|(\exp tA)x\|^2.$$

Using the condition (C), this gives for $t \to \infty$:

$$\int_0^\infty \|j_Q(\exp tA)x\|^2\, dt = \|x\|^2.$$

Hence the map $x \mapsto j_Q(\exp tA)x$ is an isometry, hence admits an isometric extension $X \to L^2(\mathbb{R}^+, X_Q)$. Hence this extension, denoted abusively $x \to j_Q(\exp tA)x$, is a causal filter, defined on X, and adapted to any white noise N with covariance $\delta_0(t-s)Q$. Clearly the restiction ξ of $\hat{\xi} = j_Q(\exp tA)*N$, to the subspace Dom A of X, satisfies (i) and (iii). Hence we show only $D\xi - A^T\xi = N$.

The notation $h(t)x = j_Q(\exp_+ tA)x$ is used below $\forall x \in X$. For any $x \in \text{Dom } A$, $h(t)x$ is a distribution on the line, with values in X_Q, solution of

$$D(h(t)x) - A(h(t)x) = D(h(t)x) - h(t)Ax$$

$$= \delta_0(t) \otimes (j_Q x).$$

By translation, this gives for arbitrary fixed real u:

$$D_t(h(t-u)x) - h(t-u)Ax = \delta_u(t) \otimes (j_Q x).$$

Hence for arbitrary $\varphi \in \mathscr{D}(\mathbb{R})$, $x \in \text{Dom } A$,

$$\langle (D\xi)_\varphi - (A^T\xi)_\varphi, x\rangle = \langle -\xi_{D\varphi}, x\rangle - \langle \xi_\varphi, Ax\rangle$$

$$= \left\{N_u, -\int (D\varphi)(t)h(t-u)x\, dt - \int \varphi(t)\, dt\, h(t-u)(Ax)\right\}$$

$$= \left\langle N_u, \left(\int \delta_u(t)\varphi(t)\, dt\right) \otimes j_Q x\right\rangle$$

$$= N_u(\varphi(u) \otimes j_Q x) = \langle N_\varphi, x\rangle.$$

This proves (ii); hence the converse assertion is proved.

2.4 Application to finite-dimensional processes

In particular, Doob's result can be deduced from the direct and the converse assertion, using the following fact:

An $n \times n$ real matrix A is asymptotically stable iff there exists an Euclidean structure X on $\mathbb{R}^n$ such that $t \to \exp tA$ is a contraction semigroup in X, satisfying the condition (C).

The condition is clearly sufficient. Conversely, if A is asymptotically stable, then

$$C = \int_0^\infty e^{tA} e^{tA^T}\, dt$$

is a symmetric positive regular $n \times n$ matrix satisfying $AC + CA^T = -1$. Therefore,

$$D(\langle Ce^{tA^T}x, e^{tA^T}x\rangle)$$

$$= \langle (CA^T + AC)e^{tA^T}x, e^{tA^T}x\rangle$$

$$= -\|(\exp tA^T)x\|^2 \leqslant 0.$$

Hence $\forall t \geqslant 0$, $(\exp tA^T)$ is a contraction in $\mathbb{R}^n$ endowed with the scalar product $\langle Cx, y\rangle$.

2.5. Expression of spectral densities

The notations of the converse assertion are used. Then for arbitrary $x \in X$, the function $p \to j_Q (A - p)^{-1}x$, holomorphic for $\operatorname{Re} p > 0$, belongs to the Hardy class $H^+(X_Q)$. If $w \to j_Q (A - i\omega - 0)^{-1}x$ denotes the boundary value of this function, the following equality holds in $L^1(\mathbb{R}, dw)$:

$$\langle S_{\hat{\xi}}(\omega)x, x\rangle = (\| j_Q (A - i\omega - 0)^{-1}x\|_Q)^2. \tag{2.8}$$

Proof: (a) First we show

$\operatorname{Re} p > 0$ and $x \in X$

$$\Rightarrow \int_0^\infty e^{tA} e^{-pt} x\, dt = -(A - p)^{-1}x. \tag{2.9}$$

In fact, if $\hat{u}(p)$ denotes the lhs of the last equality, $\hat{u}(p)$ is the Laplace transform (LT) of $u(t) = (\exp tA)x$. Since $\hat{u}(p)$ is a linear and continuous function of the argument $x \in X$, $\hat{u}(p)$ defines a linear and continuous operator of the complexification X^c of X. In particular, for $x \in \operatorname{Dom}(A)$, $u(t)$ is a solution of the initial value problem

$$Du(t) - Au(t) = 0 \quad \text{for } t > 0, \quad u(0) = x.$$

Hence by LT: $\hat{u}(p)(p - A) = x$, or $\hat{u}(p) = (p - A)^{-1}x$ for $x \in \operatorname{Dom} A$. Finally, (2.9) follows by continuous linear extension.

(b) The point (a) uses only the inclusion of the semiplane $\operatorname{Re} p > 0$ in the resolvent set $\operatorname{Res} A$ of A. The additional L^2 properties proved in 2.3 are used below. Let (x_n) be a sequence in $\operatorname{Dom} A$ converging to $x \in X$ and $\epsilon > 0$. Using (a),

$$\int_0^\infty j_Q e^{tA} e^{-i\omega t} e^{-\epsilon t} x\, dt = -j_Q (A - i\omega - \epsilon)^{-1}x.$$

The norm of $h(t)(x - x_n) = j_Q(\exp tA) \times (x - x_n) \in L^2(\mathbb{R}^+, X_Q)$ is $\|x - x_n\|$. For any fixed $\epsilon > 0$, the sequence of functions $\omega \to j_Q (A - i\omega - \epsilon)^{-1}x_n$ converges to $\omega \to j_Q (A - i\omega - \epsilon)^{-1}x$ in $L^2(\mathbb{R}, X_Q)$.

Hence,

$$\forall \epsilon > 0, \quad \forall x \in X, \quad \int j_Q e^{tA} e^{-i\omega t} e^{-\epsilon t} x\, dt$$
$$= -j_Q (A - i\omega - \epsilon)^{-1}x.$$

This means that $\forall x \in X$, the function $p \mapsto j_Q (A - p)^{-1}x$ belongs to the Hardy class $H^+(X_Q)$. By Plancherel's Theorem, this function has a boundary value; this boundary value denoted by $j_Q (A - i\omega - 0)^{-1}x$ is the FT of $h(t)x$.

(c) Since $\hat{\xi}$ is physically realized by filtering N, using the causal filter $x \mapsto h(t)x$ defined on X, (2.8) follows from (1.14).

2.6. Comments concerning Formula (2.8)

(a) The scalar products of the complexified spaces X^c and X_Q^c are denoted, respectively, $(\ ,\ )$ and $(\ ,\ )_Q$. These complexifications are viewed below as real vector spaces. By complexification of (2.8),

$$\forall x \in X^c, \quad (S_{\hat{\xi}}(\omega)x, x)$$
$$= \| j_Q (A - i\omega - 0)^{-1}x\|_Q^2$$
$$= ((A - i\omega + 0)^*)^{-1} Q ((A - i\omega - 0)^{-1}x, x). \tag{2.10}$$

(b) If $\operatorname{Res} A$ contains some open interval I of the imaginary axis for arbitrary $x \in X^c$, the function $\langle S_{\hat{\xi}}x, x\rangle$ restricted to I is represented by $\langle Fx, x\rangle$, where $F: I \to L(X^c)$ is continuous and defined by $F(\omega) = (A - i\omega)^{*-1} Q (A - i\omega)^{-1}$. In particular, if as in the finite-dimensional case, $\operatorname{Res} A$ contains the imaginary axis, then

$$S_{\hat{\xi}}(\omega) = (A - i\omega)^{*-1} Q (A - i\omega). \tag{2.11}$$

3. THE REALIZABILITY THEOREM

In this section, the notations of 2.3 are systematically used. In particular, $\hat{\xi}$ denotes any c.p. constructed as in 2.3.

3.1 Definition of realizability

(a) A linear observation of some c.p. $\hat{\xi}$ is defined by some $B \in L(Y, X)$, where Y denotes a l.c.H.s. The result of this observation is the c.p. $B^T\hat{\xi}$ defined as follows:

$$\forall t, \quad \forall y \in Y, \quad \langle B^T\hat{\xi}_t, y\rangle = \langle \hat{\xi}_t, By\rangle.$$

(b) A c.p. (g_t), with values l.p. on some l.c.H.s. Y is called realizable if (g_t) is isonomic with some linear observation B of some c.p. $\hat{\xi}$. The number $\dim X$ is called the dimension of the realization $(B, \hat{\xi})$ of (g_t).

This agrees for $\dim X$ finite with the usual definition of realizations.

3.2. The realizability theorem

For any stationary Gaussian c.p. (g_t) on the line, with linear process values on some l.c.H.s. Y, the following assertions are equivalent:

(a) g is realizable,

(b) g is physically realizable by filtering some Gaussian white noise,

(c) there exists a real Hilbert space X_Q and $H: y \to H(\omega)y$, element of $L(Y, H^+(X_Q))$ such that the following equalities hold in $L^1(\mathbb{R}, d\omega)$:

$$\forall y \in Y, \quad \langle S_g(\omega)y, y\rangle = (\|H(\omega)y\|_Q)^2.$$

Proof: Two stationary continuous Gaussian c.p. on the line, with values l.p. on the same l.c.H.s. Y, are isonomic iff they have identical spectral measures. Hence using (1.14), (b)$\Leftrightarrow$(c).

(a)$\Rightarrow$(b). Let (g_t) be a realizable c.p., and let $(\hat{\xi}, B)$ be some realization of (g_t). Since $\hat{\xi}$ is physically realized by filtering some Gaussian white noise N with the causal filter $x \to j_Q(\exp tA)x$ on X, $B^T\hat{\xi}$ is physically realized by filtering N with the causal filter $y_Q(\exp tA)B \in L(Y, L^2(\mathbb{R}, X_Q))$.

(b)$\Rightarrow$(a). Let X_Q be a Hilbert space, and let N be the Gaussian white noise obtained by identifying isometrically $L^2(\mathbb{R}, X_Q)$ with a space of Gaussian r.v. Let $g = h * N$ be a c.p. physically realizable by filtering N with $h \in L(Y, X_1)$ with $X_1 = L^2(R^+, X_Q)$. We have to find a realization $(\hat{\xi}, B)$ of g. The semigroup $\varphi(\cdot) \to \varphi^t = \varphi(t + \cdot)$ of left translation in X_1 is denoted $t \mapsto \exp tA$. Since this contraction semigroup satisfies the condition (C), $\hat{\xi}$ will be constructed using 2.3.

Since the domain of the infinitesimal generator $A = d/dt$ in X_1 is the Sobolev space $H^1(R^+, X_Q)$, the dual space $(\operatorname{Dom} A)'$ is[6] the space of all elements of $H^{-1}(\mathbb{R}, X_Q)$ supported by $[0, +\infty[$. The domain of A^T is the subspace of

Dom A, consisting of all elements vanishing at the origin, and $A^T = -D$. Hence $Q_1 = -A - A^T = 0$!! But $Q_1 \neq 0$ since $\forall \varphi \in \mathrm{Dom}\, A$, $Q_1\varphi = \delta_0 \varphi(0)$. Hence, the stochastic Hilbert space of the quadratic form $\langle Q_1 \varphi, \varphi \rangle$ on Dom A is $X_{Q_1} = X_Q$ and the associated map j_{Q_1} Dom $A \to X_{Q_1}$ is $\varphi \mapsto \varphi(0)$. Let N^1: $\mathscr{D}(\mathbb{R}) \otimes \mathrm{Dom}\, A \to L^2(\mathbb{R}, X_Q)$ be the white noise product of $j \otimes j_{Q_1}$ with the canonical injection of $L^2(\mathbb{R}) \otimes X_Q$ in $L^2(\mathbb{R}, X_Q)$. Putting $\hat{\xi} = (j_{Q_1}(\exp_+ tA))$ $*N^1$, we have (b)$\Rightarrow$(a), since for arbitrary time t, $y \in Y$, and with $h = B$,

$$\begin{aligned} \langle h^T \hat{\xi}_t, y \rangle &= \langle N^1_u, j_{Q_1}(\exp_+(t-u)A)(h(\,.\,)y) \rangle \\ &= \langle N^1_u, j_{Q_1}(h(t-u+\,.\,)y) \rangle \\ &= \langle N^1_u, h(t-u)y \rangle = \langle (N^1 * h^T)_t, y \rangle. \end{aligned}$$

4. THEOREM OF SIMULTANEOUS REALIZATION

In the last section, the following result has been proven:

4.1. Theorem of simultaneous realization

Let X_Q be a Hilbert space and let N be a Gaussian white noise, obtained by identifying isometrically $X_1 = L^2(\mathbb{R}, X_Q)$ with a space of Gaussian r.v. Then a c.p. $\hat{\xi}$ can be constructed such that for any l.c.H.s. Y and any causal filter $h \in L(Y, X_1)$ adapted to N, the c.p. $h^T * N$ physically realized by filtering N, coincides with the observation $h^T \hat{\xi}$ of $\hat{\xi}$.

4.2. Connection with finite-dimensional realizability

As is well known, if a process (g_t) with values in some Euclidean space Y is an observation of some process (ξ_t) living in some Euclidean space X, then necessarily, the spectral density of (g_t) can be written

$$S_g(w) = R(i\omega)^* R(i\omega) / |Q(i\omega)|^2 \tag{4.1}$$

with Q = real polynomial with all roots in the half-space Re $p < 0$, with R = polynomial of degree $<$ deg Q, and with coefficients in $L(Y^c, X^c)$. Conversely, if a process (g_t) with values in Y admits a spectral density of this "rational type," a finite-dimensional realization of (g_t) can be constructed easily. We show now how such realization is "imbedded" in the universal realization given by the theorem. In fact, let $h \in L(Y, L^2(\mathbb{R}^+, X)) \simeq L^2(\mathbb{R}^+, L(Y, X))$ be such that $\mathscr{F} h = R(i\omega) Q(i\omega)^{-1}$. Then $g = h * N$ for some white noise N with covariance $\delta_0(t-s) \otimes \mathrm{Id}(X)$. Hence $g = h^T \hat{\xi}$ by the theorem, where $\hat{\xi}_t$ is for all t, a linear process on $X = L^2(\mathbb{R}^+, X)$. Decomposing the rational fraction RQ^{-1} in irreducible elements, it is easy to see that h takes values in a finite-dimensional subspace X_1^{fin} of X_1, invariant for all left time translations. Hence, $h^T \xi$ is, in fact, a linear observation of the restriction ξ^{fin} of $\hat{\xi}$ to the subspace X_1^{fin} of X_1: this defines a finite-dimensional realization of g_t. The theorem of simultaneous realization permits the study of approximate realizations, according to a given probabilistic criterion. We give a simple example.

4.3. Approximate realization, according to the energy

Let N be a white noise with covariance $\delta_0(t-s)\mathrm{Id}(X)$, where X is a Euclidean space. Let $g = h^T * N$ be a process physically realized by filtering N with the causal filter $h \in X_1 = L^2(\mathbb{R}^+, \mathrm{End}\, X)$. A polarity argument[7] shows that the space $\mathscr{E}$ of elements $\in X_1$ with FT of the type $h = RQ^{-1}$ (Q = real polynomials with all roots in the half-space Re $p < 0$; R = polynomial of degree $< Q$ and with coefficients $\in X^c$), is dense in X_1. Hence there exists a sequence (h_n) in $\mathscr{E} \otimes X$ with limit h in X_1, endowed with the natural Hilbertian norm. Hence the processes $g^n = (h_n^T)\hat{\xi}$ have finite-dimensional realizations. Moreover the process (g^n, g) is stationary and at any time t,

$$\begin{aligned} E(\| g_t - g_t^n \|^2) &= E(\| (h_n - h)^T \xi_t \|^2) \\ &= (\| h_n - h \|_{X_1})^2 \to 0. \end{aligned}$$

5. EXAMPLES OF REALIZABLE RANDOM FIELD

5.1. Definition

If I denotes an open subset of $\mathbb{R}^d$, the triplet $\mathscr{D}(I) \subset L^2(I) \subset \mathscr{D}'(I)$ will be used below. Let $(c_{t,x})$ be a continuous Gaussian field on $\mathbb{R} \times I$, stationary with respect to the time translations. This field is characterized statistically by the covariance or, equivalently, by the interspectral measures

$$C_c(t; x, x') = E(c_{t+h,x} c_{h,x'}),$$

$$R(\omega; x, x') = (2\pi)^{-1} (\mathscr{F}_t C)(\omega; x, x').$$

In order to apply the previous results, the random field $(c_{t,x})$ is characterized by the following c.p. on the line, with values l.p. on $\mathscr{D}(I)$:

$$\forall t, \quad \forall \varphi \in \mathscr{D}(I), \quad \langle g_t, \varphi \rangle = \int c_{t,x} \varphi(x)\, dx.$$

For arbitrary t, $C_g(t)$ is the linear operator $\mathscr{D}(I) \to \mathscr{D}'(I)$ with integral kernel $C_c(t; x, x')$; i.e., $C_g(t)$ is the linear operator

$$\varphi \to \int C_c(t; x, y) \varphi(y)\, dy.$$

Hence $\forall \varphi \in \mathscr{D}(I)$, the following equality for measures holds:

$$\langle S_g(\omega)\varphi, \varphi \rangle = \int R_c(\omega, x, x') \times \varphi(x)\varphi(x')\, dx\, dx'.$$

By the realizability theorem, $(C_{t,x})$ is realizable iff these measures admit densities with respect to $d\omega$, and if there exists a real Hilbert space X_Q and $h \in L(\mathscr{D}(I), H^+(X_Q))$ such that the following equalities hold in $L^1(\mathbb{R}, d\omega)$:

$$\forall \varphi \in \mathscr{D}(I), \ \langle S_g(\omega)\varphi, \varphi \rangle = (\| (h\varphi)(\omega) \| X_Q)^2.$$

In order to give simple examples, we consider the particular case where $I = \mathbb{R}^d$, and where the random field $(c_{t,x})$ is stationary with respect to all translations in $\mathbb{R}^{d+1}$. A second partial FT of the covariance $C_c(t, x - x')$ produces the total FT, i.e., the spectral $\Sigma(\omega, \xi)$ of the random field $(c_{t,x})$:

$$\Sigma(\omega, \xi) = \iint (\exp(-it\omega - i\langle x, \xi \rangle)) \times C_c(t, x)\, dt\, dx.$$

5.2 A class of realizable random fields

Let X_Q be the real Hilbert space defined by the complex space $L^2(\mathbb{R}^d, \xi)^c$. Let $(c_{t,x})$ be a stationary Gaussian random field on $\mathbb{R}^{d+1}$, with spectral measure of the type

$$\Sigma_c(\omega, \xi) = (2\pi)^{d+1} |k(\omega, \xi)|^2 \, dw \, d\xi$$

for some $h(\omega, \xi) \in H^+(X_Q)$. Then the c.p. defined by $(c_{t,x})$, with values l.p. on $\mathscr{D}(\mathbb{R}^d)$ can be realized using the observation map

$$\mathscr{D}(\mathbb{R}^d) = \mathscr{D} \xrightarrow{h} H^+(X_Q)$$

$$\varphi \to k(\omega, \xi)\hat{\varphi}(\xi).$$

In fact, the Plancherel Theorem gives $\forall \varphi \in \mathscr{D}$,

$$2\pi \langle S_g(\omega)\varphi, \varphi \rangle$$
$$= (2\pi)^{-d-1} \int \Sigma(\omega, \xi) |\hat{\varphi}(\xi)|^2 \, d\xi$$
$$= \int |k(\omega, \xi)\hat{\varphi}(\xi)|^2 \, d\xi$$
$$= (\|h\varphi\|_{X_Q})^2.$$

Hence by the realizability theorem, (g_t) is realizable. For example, the spectral density (0.5) can be realized using

$$k(\omega, \xi) = (2\pi)^{-(d+1)/2} (i\omega + (1 + |\xi|^2)^{1/2})^\alpha .$$

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First-order equations of motion for classical mechanics

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A global canonical first-order equation of motion is derived for any mechanical system obeying Newton's second law. The existence of a Lagrangian is not assumed, but the properties of the canonical equation are similar to those of the Hamiltonian formulation. The choice of map F from velocity space to phase space is not determined by the condition that the first-order equation of motion be equivalent to a second-order equation on configuration space and therefore is left open to be selected on the basis of other considerations. The canonical equation is a covector or 1-form equation on the Whitney sum $T^*Q \oplus TQ$ and contains the second-order equation condition, restriction to the graph of the map F, and Newton's equation of motion in first-order form. The last is related to Newton's second-order equations by the consistency condition that the motions not lead off graph F in $T^*Q \oplus TQ$. The first-order equation of motion can be projected onto phase space if the map F can be inverted.

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I. INTRODUCTION

"One of the motivations of these works is the following: if we understand truly classical analytical dynamics, we have a chance to understand more easily quantum dynamics and to obtain new invariant tools." Lichnerowicz[1]

Newton's laws[2] describe the motions of a classical mechanical system in terms of second-order differential equations. However, for many purposes,[3] as in statistical mechanics and canonical quantization, these motions are more conveniently described by first-order differential equations, in particular those of the Hamiltonian formulation.[4] The goal of the present work is to derive a global canonical[5] first-order equation of motion for any Newtonian mechanical system, without assuming the existence of a Lagrangian.[6]

The standard derivations[7–10] of the Hamiltonian formulation from Newton's equations of motion for a system (possibly constrained) or from Euler–Lagrange equations cannot be generalized directly since these derivations depend critically upon the existence of a Lagrangian L whose derivatives $\partial L/\partial v^i$, the canonical momenta, determine the velocities completely and uniquely. Moreover, those derivations leave unanswered many questions, such as, "What is the origin of the $p \cdot v$ term in the Hamiltonian?"

The arguments given below explain the origin of that term and other features of the first-order formulation, and show that many of these features are independent of the existence of a Lagrangian. Thus even though one may end up with the Hamiltonian formalism for the important motions described by a Lagrangian, it is worthwhile to derive the canonical first-order equations without assuming a Lagrangian in order to see the roles played by other considerations in determining the features of the canonical equations.

The derivation, which is the source of the explanations, is based on the use of the one fact that we know about the Newtonian equations of motion for any mechanical system, namely, that the differential equations are second-order. This one fact leads, for instance, to the use of differential forms in the first-order equation of motion, and then to phase space, and to the appearance of the $p \cdot v$ term.

The concern here does not lie in proving that the derived canonical first-order form is unique—it is not—but rather that there are reasonable arguments applicable to all second-order equations that lead to that form. Reasonable choices have to be made at some points in the derivation, and a choice diverging from that taken here may lead to another form for first-order equations of motion.

The derivation of a global canonical first-order equation for motions satisfying any reasonably well-behaved second-order differential equation is carried out in stages. Second-order differential equations and the problem in mapping these to first-order equations are discussed in Sec. II. Section III shows how to incorporate the second-order equation condition into a first-order equation, and the final form of the canonical first-order equation is obtained in Sec. IV. Variations in the formulation are introduced in Sec. V. A brief summary and discussion are given in Sec. VI.

II. THE SECOND-ORDER EQUATION CONDITION

The set of possible positions q_Q of a mechanical system is assumed to be in bijective correspondence with a differentiable manifold[11] Q, called configuration space. Furthermore, general differentiable manifold structures must be considered, since Q need not be diffeomorphic to a Cartesian space without excluding such a simple case as motion on a sphere. Locally, each point q_Q is represented by coordinate functions $\{q_Q^i\} = (q_Q^1, q_Q^2, \ldots, q_Q^N)$.

Newton's laws of motion involve a relation, the second-order equation of motion, that determines the acceleration $\{d^2 q_Q^i/dt^2\}$ in terms of the velocity $\{dq_Q^i/dt\}$ and the configuration $\{q_Q^i\}$; it is assumed in the following that this relation is given. Our objective is to write this second-order equation of motion in canonical first-order form, so we begin with an examination of second-order equations on a manifold.[12]

An *(ordinary) first-order (differential) equation*[13] on a manifold Q (also called a vector field on Q or a cross section of TQ) is a differentiable map

$$\Phi:\ Q \to TQ\ \ [\text{or } \Phi:\ \mathscr{F}(Q) \to \mathscr{F}(Q)] \tag{1}$$

that satisfies $\tau_Q \cdot \Phi = id_Q$. A first-order equation on the tangent bundle TQ does not give, in general, an ordinary second-order differential equation on Q. The necessary and sufficient condition[14] that a first-order equation Σ on TQ must satisfy in order that it be an *(ordinary) second order (differential) equation* on Q,

$$\tau_{Q*} \cdot \Sigma = id_{TQ}, \tag{2}$$

restricts the image of Σ to the submanifold $T^2Q \subset TTQ$ and is called the *second-order equation condition*.[15] It holds also for generalized second-order differential equations (in the sense of the title of Dirac's pioneering paper[16]).

We now confront the problem of determining the *first-order equation of motion*, the equation that determines the first-order differential equation given the second-order differential equation on Q,

$$X_2:\ TQ \to T^2Q \subset TTQ. \tag{3}$$

The solution of either a second- or a first-order equation of motion is a first-order equation X on some space: the second-order equation condition distinguishes them. A second-order equation of motion involves the second-order equation condition and a separate equation for the other components of X, while a first-order equation of motion is a *single* equation for X.

A. The second-order equation condition mapped to a first-order equation

The properties of the manifold M, on which the first-order equation X_1: $M \to TM$ exists, will be specified as we proceed by examining the conditions that M must satisfy in view of our goal.

Since we are transforming second-order to first-order differential equations, we assume that $\dim M = 2 \dim Q$. Moreover, since the eventual aim is to determine motions on Q, the solutions of X_1 must project from M to Q, so we assume that M is a bundle with base space Q, pr: $M \to Q$.

Also, the first-order equation X_1 on M must be equivalent to the second-order equation X_2 on Q in the following sense: To each solution curve on X_2 on TQ, there is one and only one solution curve of X_1 on M such that the induced curves in Q are identical. Thus there is a map from the space of solution curve points[17] of X_2, F: $TQ \to M$, such that $\mathrm{pr} \cdot F = \tau_Q$ (so F is fiber-preserving).

One half of the first-order equation on M is given always by a mapping of the second-order equation condition,

$$\mathrm{pr}_* \cdot X_1 \cdot F = id_{TQ}: \tag{4}$$

the part $\mathrm{pr}_* \cdot X_1$ of the first-order equation on M is given by the second-order equation condition to be the pre-image under F of $\tau_M \cdot X_1$.

However, without knowing the map F, we cannot write down that part, $\mathrm{pr}_* \cdot X_1$, of the first-order equation on M that corresponds to the second-order equation condition. Nevertheless, since we know, at every point on TQ, the form of $\mathrm{pr}_* \cdot X_1$, and since M and TQ are bundles over Q, that part of the first-order equation can be given (essentially) by $\tau_{Q*} \cdot X_2 = id_{TQ}$ on the generalized Whitney sum[18] $W_0 = M \oplus TQ$ with canonical projection pr_i $(i = 1, 2)$ on the ith factor.

The differential equations X_2 on TQ and X_1 on M induce a map

$$X:\ \text{graph } F \subset M \oplus TQ \to T(M \oplus TQ) \tag{5}$$

that projects, by pr_{1*} and pr_{2*}, to X_1 on M and X_2 on TQ, respectively, and is tangent to $W_1 = \text{graph } F$. Therefore X satisfies the consistency condition that it does not generate curves leading off the constraint submanifold W_1.

The second-order equation condition can be applied at every point of $M \oplus TQ$, in which case it holds in particular on graph F. The condition for *any* first order differential equation on $M \oplus TQ$

$$X:\ M \oplus TQ \to TM \oplus T^2Q \subset T(M \oplus TQ) \tag{6}$$

to project by pr_{2*} to a second-order equation on Q can be written as

$$\mathrm{pr}_* \cdot \mathrm{pr}_{1*} \cdot X = \mathrm{pr}_2, \tag{7}$$

in which the left-hand side involves $\mathrm{pr}_{1*} \cdot X$, the part of X that corresponds to the first-order equation on M. Thus this form of the second-order equation condition is useful for the problem at hand. Moreover, invoking the second-order equation condition in a form that holds throughout $M \oplus TQ$ allows the addition of components to the equation of motion that restricts that equation to graph F.

[If $M = T^*Q$, this form of the second-order equation condition appears remarkably similar,[19] if one takes into account the directions of the maps, to the definition of the canonical 1-form on $T^*Q \oplus TQ$ (the pullback of the canonical 1-form on T^*Q),

$$\theta_{\oplus} = \mathrm{pr}_1^* \cdot \mathrm{pr}^* \cdot \mathrm{pr}_1. \tag{8}$$

The present work arise from a study of the reasons for this similarity, in particular an investigation of whether or not the second-order equation condition (7) led directly to the appearance of the canonical 1-form (8) in the canonical equation of motion.]

Now we examine what features of the first-order equation of motion follow from the second-order equation condition.

III. THE SECOND-ORDER EQUATION CONDITION AS PART OF THE FIRST-ORDER EQUATION OF MOTION

Our interest lies in a *single* equation for $\mathrm{pr}_{1*} \cdot X$, of which the relation (7) is one part. The map pr_* can be removed from $\mathrm{pr}_{1*} \cdot X$ only by taking the left-hand side as the argument of a form: for any element α of T_q^*Q, with $q = \tau_Q \cdot \mathrm{pr}_2 \cdot \tau_{W_0} \cdot X$, the second-order equation condition on $M \oplus TQ\,|_{\tau_{W_0} \cdot X}$ may be written as

$$\langle \mathrm{pr}_1^* \cdot \mathrm{pr}^* \cdot \alpha | X \rangle = \langle \alpha | \mathrm{pr}_2 \rangle \quad \text{for every } \alpha \in T_q^*Q. \tag{9}$$

[Note the appearance, for $M = T^*Q$ and $\alpha = \mathrm{pr}_1$, of $\langle p | v \rangle$ on one side, and the canonical 1-form (8) on the other, of this part of the first-order equation of motion.]

Our final concern is a first-order equation on M, so we transform (9) so it involves elements on T^*M. Since each $\beta = \mathrm{pr}^* \cdot \alpha$ is an element of, and the set generated by all $\alpha \in T^*Q$ spans,

$$H^*M = \{\gamma \in T^*M \text{ such that } \langle \gamma | Y_1 \rangle = 0$$

$$\text{for every } Y_1 \in TM \text{ such that } \mathrm{pr}_* \cdot Y_1 = 0\}, \tag{10}$$

a bijective map

$$\sigma\colon H^*M \to T^*Q\colon \gamma \mapsto \sigma\cdot\gamma \tag{11}$$

with $\mathrm{pr}^*\cdot\sigma = id_{H_*M}$ is defined by

$$\langle \gamma | Y_1 \rangle = \langle \sigma\cdot\gamma | \mathrm{pr}_* \cdot Y_1 \rangle \quad \text{for every } Y_1 \in TM. \tag{12}$$

Thus replacing α by $\sigma\cdot\beta$ in (9) gives

$$\langle \mathrm{pr}_1^* \cdot \beta | X \rangle = \langle \sigma\cdot\beta | \mathrm{pr}_2 \rangle \quad \text{for every } \beta \in H^*M \tag{13}$$

for the second-order equation condition.

This equation is but one half of the first-order equation of motion, as it appears on $M \oplus TQ$, for $\mathrm{pr}_{1*} \cdot X$. We want a single equation for $\mathrm{pr}_{1*} \cdot X$, so we modify the second-order equation condition (13) further until there is an obvious generalization to the desired form.

The appearance of 1-forms in (13), resulting from the map pr_* in (7), suggests rewriting the second-order equation condition as an equality between 1-forms restricted to evaluation on a vector subspace; the obvious generalization comes from removing the restriction.

The complete 1-form, whose vanishing is the equation of motion for X, is here called the *motion 1-form (for X)*:

$$\mu\colon \mathfrak{X}(W_0) \to T^*W_0. \tag{14}$$

That part of the motion 1-form that is homogeneous in X is the *inertial 1-form* and the remainder, that part independent of X, is the negative of the *dynamical 1-form*.

At this point in the development of the argument for the canonical first-order equation of motion, it is possible to see the general shape of that argument. All told, there are $4N = 4 \times \dim Q$ component equations: there are N components to the second-order equation condition, N component equations defining the map, and $2N$ component equations for the velocities of the coordinates, other than those of Q, in M, and in TQ. Let $\{q^i, p_j, v^k\}$ be coordinate functions on $T^*Q \oplus TQ$, and $\{\dot q^i, \dot p_j, \dot v^k\}$ be the corresponding components of $X \in T(T^*Q \oplus TQ)$. The basis 1-forms that appear in the motion 1-form (14) can be taken locally to be dq^i and dv^i and, since our concern lies in 1-forms like the α of (9), those, dp_i, on T^*Q. To obtain a global 1-form then, we can identify M with T^*Q and form linear combinations (inner products) of the dq^i and the dv^i with p_i and $\dot p_i$ and of the dp_i with v^i, $\dot q^i$, and $\dot v^i$. The additional relations needed are provided by the consistency condition that X be tangent to graph F; this relates $\dot v^i$ to $\dot p^i$. Dimensional analysis indicates that the motion 1-form can involve the combinations (a) $\dot p_i dq^i$, (b) $p_i dv^i$, (c) $v^i dp_i$, and (d) $\dot q^i dp_i$. The second-order equation condition is satisfied if the only terms in dp_i in the motion 1-form are [(c) − (d)], and (b) and (c) combine in [(b) + (c)] to give $d\langle p|v\rangle$. Furthermore, (a) and (d) combine by subtraction into the simple form $i(X)\cdot\mathrm{pr}_1^*\cdot\omega_Q$, where ω_Q is the canonical 2-form on T^*Q. Thus armed only with the knowledge that we want a single equation for X and that this be equivalent to a second-order equation, we arrive at

$$\mu(X) = i(X)\cdot\mathrm{pr}_1^*\cdot\omega_Q - d\langle p|v\rangle + \text{terms in } dq^i \text{ and } dv^i \text{ defining the map } F \text{ and } \dot p_i(q,p,v), \tag{15}$$

with the expressions for the $\dot p_i(q,p,v)$'s coming from the given second-order equations (the $\dot v^i$'s) by means of the consistency condition.

We now return to the general problem. Because the terms in the second-order equation condition (13) are linear and homogeneous in β, two possibilities for the motion 1-form come to mind, one involving derivatives and another involving a 2-form. We examine each possibility in turn.

A. The second-order equation condition in terms of derivatives of a form

The second-order condition (13) can be replaced by an equation that involves N linearly independent derivative operators that act only on the covector part in which the β's are replaced by a differential 1-form $\phi\colon M \to H^*M$ (with M assumed to be such that a 1-form with the properties listed below exists). Furthermore, in order that the final form of the second-order equation of motion can be generalized to the complete equation of motion, ϕ must vary sufficiently over M to give $2N$ independent equations after suitable differentiations: thus $d\phi$ must be nondegenerate. In this case, $\sigma\cdot\phi\colon M \to T^*Q$ is a diffeomorphism. Thus we replace $\sigma\cdot\beta$ in (13) with $\sigma\cdot\phi\cdot\mathrm{pr}_1$.

Because the values of ϕ lie in H^*M, the appropriate derivative operators are Lie derivatives with respect to elements of the N-dimensional vector space

$$V_1 = \{Z \in T(M \oplus TQ) \quad \text{such that } \mathrm{pr}_{2*} \cdot Z = 0\}, \tag{16}$$

derivative operators that we denote collectively by $\mathbf{L}_{V_1}$. Since $\mathbf{L}_{V_1}\cdot(f\cdot\mathrm{pr}_2) = 0$ for every f in $\mathscr{F}(TQ)$, the second-order equation condition (13) is equivalent to[20]

$$\begin{aligned}\langle \mathbf{L}_{V_1}\cdot\mathrm{pr}_1^*\cdot\phi\cdot\mathrm{pr}_1 | X \rangle &= \mathbf{L}_{V_1}\cdot\langle \sigma\cdot\phi\cdot\mathrm{pr}_1 | \mathrm{pr}_2 \rangle \\ &= -i(V_1)\cdot i(X)\cdot d\theta'_0 = i(V_1)\cdot d\langle \sigma\cdot\phi\cdot\mathrm{pr}_1 | \mathrm{pr}_2 \rangle,\end{aligned} \tag{17}$$

with

$$\theta'_0 = \mathrm{pr}_1^*\cdot\phi\cdot\mathrm{pr}_1 \quad \text{and} \quad \omega'_0 = -d\theta'_0. \tag{18}$$

This suggests, under the generalization procedure described above (14), that the equation of motion is

$$i(X)\cdot\omega'_0 = d\langle \sigma\cdot\phi\cdot\mathrm{pr}_1 | \mathrm{pr}_2 \rangle + \lambda', \tag{19}$$

with $i(V_1)\cdot\lambda' = 0$, as it contains the second-order equation condition for any such λ'. In particular, for $M = T^*Q$ and $\sigma\cdot\phi = id_{T_*Q}$, one obtains that ω'_0 is the canonical 2-form and that

$$i(X)\cdot\omega'_0 = d\langle \mathrm{pr}_1 | \mathrm{pr}_2 \rangle + \lambda', \tag{20}$$

so it can be argued that the canonical 2-form and the $p\cdot v$ term in the Hamiltonian arise from the second-order equation condition.

We return to determine λ' after considering the use of a 2-form in the second-order equation condition.

B. The second-order equation condition in terms of a 2-form

The problem of stripping the map pr_* from X in the second-order equation condition (7) shows that the single equation of motion for X involves X as the argument of a differential form, i.e., of exterior products of elements of $T^*(M \oplus TQ)$. Since the equation of motion is to determine the first-order equation $\mathrm{pr}_{1*} \cdot X$, these elements are pullbacks by pr_1^* of elements of T^*M. The solution of the equation of motion gives $\mathrm{pr}_{1*} \cdot X$ in terms of $\tau_{W_0} \cdot X$, so the consequence of evaluating the form on X in terms of $\tau_{\omega_0} \cdot X$ must contain the same information, and thus have the same number of independent components, as $\mathrm{pr}_{1*} \cdot X$. Therefore the form is the pullback by pr_1^* of a nondegenerate 2-form ω_M on M (which is assumed to exist). Then since $\omega_0 = \mathrm{pr}_1^* \cdot \omega_M \cdot \mathrm{pr}_1$ is nondegenerate on V_1, the values of $i(V_1) \cdot i(X) \cdot \omega_0$ are equal, by the second-order equation condition (7), to linear combinations of the N linearly independent values of $\langle \sigma \cdot H^*M \,|\, \mathrm{pr}_2 \rangle$. These linear combinations can be calculated once ω_M is chosen.

We conclude, from arguments similar to those used in Subsec. A, that it is appropriate to take $i(X) \cdot \omega_0$ as the inertial 1-form, and that the dynamical 1-form δ involves N linearly independent combinations of the $\langle \sigma \cdot H^*M \,|\, \mathrm{pr}_2 \rangle$.

Before we consider the properties of the dynamical 1-form δ, we note that the nondegenerate 2-form can be chosen at this point on the basis of considerations other than those discussed later in Sec. IV. For example, one can require that the equation of motion be such that, about any point in $M \oplus T^*Q$, there be a coordinate system $\{m^\alpha\}$ on M, called canonical, in terms of which the equation of motion has the velocity components isolated on one side. Thus in those coordinates, the 2-form ω_M has the form $\omega_M = dy_i \wedge dx^i$ for $\{y_i, x^j\} = \{m^\alpha\}$. Equivalently, by the theorem of Darboux, $d\omega_M = 0$, so, at least locally, there exists a 1-form θ_M such that $\omega_M = -d\theta_M$. Thus in this case we can set [cf. Eq. (18)], at least locally, $\phi = \theta_M$.

An alternative formulation, equivalent to that obtained by assuming the existence of canonical coordinates, is given by requiring that ω_M defines an R-bilinear bracket, the Poisson bracket

$$\{f, g\} = -i(Z_f) \cdot i(Z_g) \cdot \omega_M \tag{21}$$

that satisfies Jacobi's identity, where f and g lie in $\mathscr{F}(M)$ and $i(Z_h) \cdot \omega_M = dh$. (This makes the Poisson brackets into a Lie algebra.) An ω_M satisfying these conditions is closed,[21] so the arguments of the last paragraph apply. [Note that

$$-i(Z_f) \cdot i(X_1) \cdot \omega_M = \dot{f}, \tag{22}$$

even if $i(X_1) \cdot \omega_M$ is not an exact 1-form.]

We return now to the general problem to see how to determine the dynamical 1-form δ.

IV. THE CANONICAL FIRST-ORDER EQUATION

The motion 1-form $i(X) \cdot \omega_0 - \delta$ of Sec. IIIB must yield zero when evaluated on any vector $Y \in T_y\ (M \oplus TQ)$ at every point y in $M \oplus TQ$. The dynamical 1-form δ is determined in part by evaluating $i(X) \cdot \omega_0$ for a given ω_M on those Y's in V_1 and imposing the second-order equation condition. Further information about δ can be obtained by considering the primary constraint submanifold (Subsec. A). This information can be combined with the second-order equation condition to provide a basis for the choice of ω_M (Subsec. B). Finally, the dynamics can be introduced to complete the derivation of the canonical first-order equation of motion (Subsec. C).

A. The primary constraint submanifold

Since $\omega_0 = \mathrm{pr}_1^* \cdot \omega_M$, for any vector Y in

$$V_2 = \{Z \in T(M \oplus TQ), \text{ such that } \mathrm{pr}_{1*} \cdot Z = 0\}, \tag{23}$$

the dynamical 1-form must satisfy $\delta(Y) = 0$ if the motion 1-form is to be zero. However, this relation need hold only on the solution subspace of $M \oplus TQ$, graph F, or the *primary constraint submanifold* in the terminology of Bergman,[22] and indeed, defines that subspace if the dynamical 1-form δ is such that

$$\text{graph } F = \{w \in M \oplus TQ, \text{ such that } \delta(Y)(w) = 0 \text{ for every } Y \text{ in } V_2\}. \tag{24}$$

A motion 1-form involving a dynamical 1-form δ with this property could contain complete information about the first-order equation of motion. That part of a δ giving graph F can be introduced in the following way.

Because δ is a 1-form, we want a 1-form that distinguishes the points w of graph F, which satisfy $\mathrm{pr}_1 \cdot w = F \cdot \mathrm{pr}_2 \cdot w$, from others in $M \oplus TQ$. For any w in $M \oplus TQ$, $\mathrm{pr}_1 \cdot w$ and $F \cdot \mathrm{pr}_2 \cdot w$ are points in M on the same fiber of pr, so we introduce a 1-form $\psi: M \to T^*M$ that distinguishes points on the same fiber in M (and thus gives verticle bundle coordinates on M). Thus an appropriate ψ satisfies, for $Y_1 \in TM$,

$$\langle \psi | Y_1 \rangle = 0 \text{ if } \mathrm{pr}_* \cdot Y_1 = 0, \quad \neq 0 \text{ if } \mathrm{pr}_* \cdot Y_1 \neq 0. \tag{25}$$

The σ of (11) and (12) then gives the diffeomorphism $\sigma \cdot \psi$: $M \to T^*Q$ with which we can introduce bundle coordinates on M:

$$q_1^i = q_Q^i \cdot \mathrm{pr} \quad \text{and} \quad m_i = \left\langle \sigma \cdot \psi \,\middle|\, \frac{\partial}{\partial q_Q^i} \right\rangle. \tag{26}$$

There are 1-forms, namely,

$$\sigma \cdot \psi \cdot \mathrm{pr}_1 - \sigma \cdot \psi \cdot F \cdot \mathrm{pr}_2 \tag{27}$$

and

$$\mathrm{pr}_1^* \cdot \psi \cdot \mathrm{pr}_1 - \mathrm{pr}_2^* \cdot F^* \cdot \psi \cdot F \cdot \mathrm{pr}_2, \tag{28}$$

that are zero only on the points of graph F. Neither of these is suitable, however, as the desired part of the dynamical 1-form δ, since the first is not an element of $T^*(M \oplus TQ)$ while both terms in the second give zero evaluated on any Y in V_2 [cf. Eq. (24)]. Thus we must refine our argument to get a 1-form on $M \oplus TQ$ that mimics the conditions for graph F given by the 1-forms (27) and (28).

For this purpose, we investigate the subspace V_2. We can associate with each Y in V_2 a unique v in TQ as follows: We express any F in $\mathscr{F}(M \oplus TQ)$ in terms of a smooth function F_1 in $\mathscr{F}(M \times TQ)$ by

$$F(w) = F_1(\mathrm{pr}_1 \cdot w,\ \mathrm{pr}_2 \cdot w) \quad \text{for } w \in M \oplus TQ. \tag{29}$$

Then for every v in TQ, the *vertical lift* at w in $M \oplus TQ$,

$$\xi_w:\ T_{\tau_Q \cdot \mathrm{pr}_2 \cdot w} Q \to T_w(M \oplus TQ):\ v \mapsto \xi_w(v), \tag{30}$$

is defined by

$$\xi_w(v) \cdot F = \frac{d}{d\lambda} F_1(\mathrm{pr}_1 \cdot w,\ \mathrm{pr}_2 \cdot w + \lambda v)|_{\lambda = 0}. \tag{31}$$

[Note that although F_1 is not defined uniquely, $\xi_w(v) \cdot F$ is.] Every Y in V_2 can be written as the vertical lift of some v in TQ,

$$Y = \xi_w(v) \text{ with } w = \tau_{W_0} Y, \tag{32}$$

and an argument concerning dimensions shows that V_2 is spanned by these vertical lifts.

The existence of the vertical lift, which spans V_2, suggests that we work with the space dual to TQ, so we consider the 1-form (27). The first term is determined by its values on every vector v in TQ [corresponding to Y in V_2 by (32)], for example, at w in $M \oplus TQ$ by

$$\langle \sigma \cdot \psi \cdot \mathrm{pr}_1 \cdot w | v \rangle = \{ i(Y) \cdot d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle \}(w). \tag{33}$$

Thus [cf. (24)] an appropriate choice to replace $\sigma \cdot \psi \cdot \mathrm{pr}_1$ is $d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle$. A similar argument for a replacement for $\sigma \cdot \psi \cdot F \cdot \mathrm{pr}_2$ does not work because it does not depend on pr_1. The problem in finding an appropriate form is, in terms of natural coordinates on $M \oplus TQ$, to replace terms in dq^i_Q by terms in dv^i with the same coefficients. This suggests using the vertical lift map since it does just that. Consider, in view of (33), a 1-form λ on $M \oplus TQ$ such that, with Y and v related by (32),

$$[i(Y) \cdot \lambda](w) = \langle \sigma \cdot \psi \cdot F \cdot \mathrm{pr}_2 \cdot w | v \rangle. \tag{34}$$

(The remainder of λ is yet to be determined.) Then we have that

$$\text{graph } F = \{ w \in M \oplus TQ \text{ such that, for every } Y \text{ in } V_2,$$
$$[i(Y) \cdot (d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle - \lambda)](w) = 0 \}. \tag{35}$$

Therefore we can write the motion 1-form as

$$i(X) \cdot \omega_0 - f(d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle - \lambda), \tag{36}$$

where one part of $f \cdot \lambda$ is to be determined by the second-order equation condition applied to $i(X) \cdot \omega_0$ and, up to this point in our argument, f is any function on $M \oplus TQ$.

B. The second-order equation condition (again)

Our arguments have led us to the motion 1-form (36) with ω_0 given in terms of an arbitrary nondegenerate 2-form ω_M on M. The second-order equation condition is to be imposed by equating, for each Y in V_1, $i(Y) \cdot i(X) \cdot \omega_0$ after the substitution (7), to

$$i(Y) \cdot [f(d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle - \lambda)]. \tag{37}$$

Now the appearance of that particular exterior derivative term suggests [cf. Eq. (17)] that an appropriate choice for ω_M could lead to some simplification in the applicaton of the second-order equation condition.

To investigate this possibility, we let $\{ Y^{(i)} \}$ denote a set of local vector fields spanning V_1 around w, and $\Phi^{(i)}_\lambda$ map the flow lines of $Y^{(i)}$, with $\Phi^{(i)}_0 = id$. Then

$$\begin{aligned} i(Y^{(i)}) \cdot d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle &= \left\langle \frac{d}{d\lambda} \sigma \cdot \psi \cdot \mathrm{pr}_1 \cdot \Phi^{(i)}_\lambda \Big|_{\lambda = 0} \Big| \mathrm{pr}_2 \right\rangle \\ &= \left\langle \mathrm{pr}_1^* \cdot \mathrm{pr}^* \cdot \frac{d}{d\lambda} \sigma \cdot \psi \cdot \mathrm{pr}_1 \cdot \Phi^{(i)}_\lambda \Big|_{\lambda = 0} \Big| X \right\rangle \\ &= \langle i(Y^{(i)}) \cdot d \cdot \mathrm{pr}_1^* \cdot \mathrm{pr}^* \cdot \sigma \cdot \psi \cdot \mathrm{pr}_1 | X \rangle \\ &= - i(Y^{(i)}) \cdot i(X) \cdot d \cdot \mathrm{pr}_1^* \cdot \psi \cdot \mathrm{pr}_1; \end{aligned} \tag{38}$$

this is simply another way of expressing the second-order equation condition. A comparison of this with (17) shows that, if we take $f = 1$, $\omega_M = -d\psi$, and $i(V_1) \cdot \lambda = 0$, the second-order equation condition and the primary constraint submanifold are a consequence of the vanishing of the motion 1-form

$$i(X) \cdot \omega_0 - (d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle - \lambda). \tag{39}$$

This is identical, with the identifications $\psi = \phi$, $\omega_0 = \omega_0'$, and $\lambda = -\lambda'$, to the motion 1-form of the equation of motion (19). We use the notation of (39) in the following.

C. The dynamics (at last)

The motion 1-form (39) has been determined, in terms of the 1-form ψ of (25) and the map F, up to one part of λ, namely, that part not involved in $i(V_1) \cdot \lambda$ nor $i(V_2) \cdot \lambda$. This part of λ is determined by the dynamics of the particular mechanical system under consideration. We assume that the dynamics is known through $X_2 = \mathrm{pr}_{2*} \cdot X$ of (3).

It is the other part of X, namely, $X_1 = \mathrm{pr}_{1*} \cdot X$, that is involved in $i(X) \cdot \omega_0$. Were it known, it could be used in the motion one-form (39) to give the yet-to-be determined part of λ. It is not though, and the equation of motion does not provide directly a relation between X_2 and X_1. That relation is given by the consistency condition that the motion, as determined by X, must not lead off graph F. Thus we have that under the flow generated by X, graph F goes into graph F: the relation between X_1 and X_2 is given by equating to zero, on graph F, the Lie derivative with respect to X of a constraint form whose vanishing determines graph F. An appropriate choice for this constraint form, since it is a 1-form on $M \oplus TQ$ and the condition does not involve evaluation on vectors restricted to a subspace, is (28).

Consistency therefore requires that

$$\begin{aligned} 0 = [&- i(X) \cdot \omega_0 + (d \langle \mathrm{pr}_1^* \cdot \psi \cdot \mathrm{pr}_1 | X \rangle \\ &- \mathbf{L}_X \cdot \mathrm{pr}_2^* \cdot F^* \cdot \psi \cdot F \cdot \mathrm{pr}_2)] |_{\mathrm{graph}\, F}, \end{aligned} \tag{40}$$

or, with $\mathrm{pr}^* \cdot \sigma = \mathrm{id}$ and the second-order equation condition,

$$\begin{aligned} 0 = [&i(X) \cdot \omega_0 - (d \langle \sigma \cdot \psi \cdot \mathrm{pr}_1 | \mathrm{pr}_2 \rangle \\ &- \mathrm{pr}_2^* \cdot \mathbf{L}_{X_2} \cdot F^* \cdot \psi \cdot F \cdot \mathrm{pr}_2)] |_{\mathrm{graph}\, F}. \end{aligned} \tag{41}$$

The right-hand side, with the restriction to graph F removed, would be suitable for the motion 1-form if we can take

$$\lambda = \mathrm{pr}_2^* \cdot \mathbf{L}_{X_2} \cdot F^* \cdot \psi \cdot F \cdot \mathrm{pr}_2. \tag{42}$$

In order that this identification be possible, the 1-form on the right-hand side of (42) must satisfy on graph F, corresponding to the conditions (34) and $i(V_1) \cdot \lambda = 0$ for λ,

$$\begin{aligned} i(Y) \cdot \mathrm{pr}_2^* \cdot \mathbf{L}_{X_2} \cdot F^* \cdot \psi \cdot F \cdot \mathrm{pr}_2 |_w \\ = \langle \sigma \cdot \psi \cdot F \cdot \mathrm{pr}_2 \cdot w | v \rangle, \end{aligned} \tag{43}$$

for Y, v, and w related by (32), and

$$i(V_1) \cdot \mathrm{pr}_2^* \cdot \mathbf{L}_{X_2} \cdot F^* \cdot \psi \cdot F \cdot \mathrm{pr}_2 = 0. \tag{44}$$

Invoking $\mathrm{pr}^* \cdot \sigma = id$ and $\mathrm{pr} \cdot F = \tau_Q$ in a coordinate calculation shows that (43) is satisfied and (44) follows from $i(V_1) \cdot \mathrm{pr}_2^* = 0$.

The *canonical first-order equation of motion* is, with a given second-order equation X_2,

$$i(X)\cdot\omega_0 = d\,\langle\sigma\cdot\psi\cdot\mathrm{pr}_1|\mathrm{pr}_2\rangle - \mathrm{pr}_2^*\cdot\mathbf{L}_{X_2}\cdot F^*\cdot\psi\cdot F\cdot\mathrm{pr}_2. \tag{45}$$

The map F and the 1-form ψ are subject[23] to the restrictions $\mathrm{pr}\cdot F = \tau_Q$ and (25), respectively. Choices for F and ψ are discussed in the next section.

V. VARIATIONS IN THE FORMULATION

The 1-form $\theta_M = \psi$, appearing in the canonical 2-form $-\mathrm{pr}_1^*\cdot d\theta_M$ of the equation of motion, may be written, since $\pi_Q\cdot\sigma\cdot\psi = \mathrm{pr}$,

$$\theta_M = (\sigma\cdot\psi)^*\cdot\theta_Q\cdot(\sigma\cdot\psi), \tag{46}$$

where $\theta_Q = \pi_Q^*$ is the canonical 1-form on T^*Q. Thus $(M, Q, \mathrm{pr}, \theta_M, \sigma\cdot\psi)$ is a *special symplectic manifold*.[24] We see that such manifolds arise naturally when one introduces first-order equations of motion equivalent to second-order equations.

Taking $M = T^*Q$ with $\sigma\cdot\psi = id$ as the prototype (as we do in the rest of this section), gives the canonical equation of motion on the Whitney sum $T^*Q\oplus TQ$

$$i(X)\cdot\omega = d\,\langle\mathrm{pr}_1|\mathrm{pr}_2\rangle - \mathrm{pr}_2^*\cdot\mathbf{L}_{X_2}\cdot F^*\cdot\theta_Q\cdot F\cdot\mathrm{pr}_2, \tag{47}$$

with $\omega = \mathrm{pr}_1^*\cdot\omega_Q$ and $\omega_Q = -d\theta_Q$. The canonical equation of motion still involves the map F, which is not determined as yet.

An alternative formulation of the canonical first-order equation of motion is obtained if the second-order equation condition is imposed on X separately from the equation of motion. Then one can set [cf. (7)]

$$d\,\langle\mathrm{pr}_1|\mathrm{pr}_2\rangle = d\,\langle\mathrm{pr}_1|\pi_{Q*}\cdot\mathrm{pr}_{1*}\cdot X\rangle = d\cdot i(X)\cdot\theta_\oplus, \tag{48}$$

where $\theta_\oplus$ is the canonical 1-form (8) on $T^*Q\oplus TQ$. With this, the canonical equation of motion (47) becomes

$$\mathbf{L}_X\cdot\theta_\oplus = \mathrm{pr}_2^*\cdot\mathbf{L}_{X_2}\cdot F^*\cdot\theta_Q\cdot F\cdot\mathrm{pr}_2. \tag{49}$$

The map F may be determined through additional considerations. For example, if there is a metric g: $TQ\rightarrow T^*Q$ on Q, then one could take $F = g$ whether or not the metric g appears in a kinetic energy term.

The map F may be chosen for some mechanical systems, called conservative, so a conservation law follows immediately from the canonical equation of motion [cf. Eq. (22)]. A sufficient condition for such a conservation law is, since $i(X)\cdot i(X)\cdot\omega = 0$, that there exists a diffeomorphism F, satisfying $\mathrm{pr}\cdot F = \tau_Q$, such that $\mathbf{L}_{X_2}\cdot F^*\cdot\theta_Q\cdot F$ be exact,[25] say, equal to the differential of L: $TQ\rightarrow R$. In this case, the conservation law is

$$\mathbf{L}_X\cdot(\langle\mathrm{pr}_1|\mathrm{pr}_2\rangle - L\cdot\mathrm{pr}_2) = 0, \tag{50}$$

and the equation of motion is

$$i(X)\cdot\omega = dD, \tag{51}$$

with the *dynamical function D* given by

$$D: T^*Q\oplus TQ\rightarrow R : w\mapsto\langle\mathrm{pr}_1\cdot w|\mathrm{pr}_2\cdot w\rangle - L\cdot\mathrm{pr}_2\cdot w. \tag{52}$$

[This differs from the Hamiltonian by being a function of the independent variables $\{q^i, p_j, v^k\}$.] This equation of motion can be written also as

$$\mathbf{L}_X\cdot\theta_\oplus = d\cdot L\cdot\mathrm{pr}_2 \tag{53}$$

if the second-order equation condition is imposed separately on X. Furthermore, the map F is [cf. Eq. (24)] the fiber derivative of L:

$$F = \mathbf{F}L: TQ\rightarrow T^*Q, \tag{54}$$

where

$$\langle\mathbf{F}L\,(\bar v)|v\rangle = \frac{d}{d\lambda}L\,(\bar v+\lambda v)\Big|_{\lambda=0}. \tag{55}$$

The components of the equation of motion (51) are, in natural bundle coordinates and with

$$X = \dot q^i\frac{\partial}{\partial q^i} + \dot p_i\frac{\partial}{\partial p_i} + \dot v^i\frac{\partial}{\partial v^i}, \tag{56}$$

$$\dot q^i = v^i, \quad \dot p_i = \frac{\partial L\,(q, v)}{\partial q^i} \tag{57}$$

and

$$p_i = \frac{\partial L\,(q, v)}{\partial v^i}. \tag{58}$$

These equations are completely equivalent to the second-order classical Euler–Lagrange equations

$$\frac{d}{dt}\left[\frac{\partial L\,(q,\dot q)}{\partial\dot q^i}\right] - \frac{\partial L\,(q,\dot q)}{\partial q^i} = 0. \tag{59}$$

And this is true even in the case in which the momenta-defining equations (58) cannot be solved for every component v^i of the velocity, i.e., when the Hessian $\det(\partial^2L/\partial v^i\partial v^j)$ is zero and the Lagrangian is said to be *degenerate*.

We now consider other formulations on graph F, T^*Q, and finally, TQ.

A. The first-order equation of motion on graph F

The fact that one needs to impose the condition that X be tangent to graph F, in addition to the equation of motion which is not satisfied off graph F, suggests the development of an equation of motion on graph F alone.

For this purpose, we introduce the inclusion map

$$j:\ \text{graph } F\rightarrow T^*Q\oplus TQ \tag{60}$$

and the map

$$\bar F:\ TQ\rightarrow\text{graph } F:\ v\mapsto(v, F\cdot v), \tag{61}$$

which is assumed to be smooth so $\bar F$ is a diffeomorphism. This map satisfies the relations

$$\mathrm{pr}_2\cdot j = \bar F^{-1}\ \text{ and }\ F = \mathrm{pr}_1\cdot j\cdot\bar F. \tag{62}$$

The condition that X be tangent to graph F is

$$X = j_*\cdot\bar F_*\cdot\mathrm{pr}_{2*}\cdot X =: j_*\cdot X_F. \tag{63}$$

The motion 1-form for the equation of motion (47) may be pulled back to graph F by j^*: it becomes

$$i(X_F)\cdot\bar j^*\cdot\omega_Q\cdot\bar j - d\cdot\langle F\cdot\bar F^{-1}|\bar F^{-1}\rangle + (\bar F^{-1})^*\cdot\mathbf{L}_{X_2}\cdot F^*\cdot\theta_Q\cdot\bar j, \tag{64}$$

where $\bar j = \mathrm{pr}_1\cdot j$.

Although the motion 1-form (64) gives an equation of motion on graph F, it cannot give the same amount of information as (47) since the latter must hold when evaluated on any vector in $T(T^*Q \oplus TQ)$, whereas the former can be evaluated only on vectors in the proper subspace $T(\text{graph } F)$ of that. The missing information is, of course, the defining equation for graph F, not[26] the second-order equation condition.

B. The first-order equation of motion on T^*Q

Because of the directions of the maps, in general, the motion 1-form on $T^*Q \oplus TQ$ cannot be pulled back to T^*Q. Instead, since there is a nondegenerate 2-form on T^*Q, one can project the solution X of the equation of motion to T^*Q, $X_1 = \mathrm{pr}_{1*} \cdot X$, and determine the equation of motion that X_1 satisfies. An example of this procedure when F is not a diffeomorphism is given in the following paper.[27]

The equation of motion on $T^*Q \oplus TQ$ can be transferred without difficulty to T^*Q if F is a diffeomorphism. In that case, $\mathrm{pr}_1 \cdot j$ is a diffeomorphism and the equation of motion (64) can be pulled back to T^*Q by $[(\mathrm{pr}_1 \cdot j)^{-1}]^*$ to give

$$i(X_1)\cdot\omega_Q = d\,\langle id\,|F^{-1}\rangle - F^{-1*}\cdot \mathrm{L}_{X_2}\cdot F^*\cdot\theta_Q, \qquad (65)$$

which includes the second-order equation condition. For a conservative system, this gives the usual Hamiltonian formulation with Hamiltonian $H = [(\mathrm{pr}_1 \cdot j)^{-1}]^* \cdot j^* \cdot D$ and the second-order equation condition taking the component form $\dot{q}^i = \partial H/\partial p_i$.

C. The canonical equation of motion pulled back to TQ

The equation of motion on graph F given by the motion 1-form (64) can be pulled back to TQ by $\overline{F}^*$. (Alternatively, of course, X may be projected by pr_{2*} to TQ. By our construction of the canonical equation for X, that must give just X_2.)

The pullback of the motion 1-form (64) is

$$i(X_2 - \mathrm{pr}_{2*}\cdot X)\cdot d\cdot F^*\cdot\theta_Q\cdot F \qquad (66)$$

by (2) since X_2 was assumed to satisfy the second-order equation condition. Therefore, if F is a diffeomorphism, so $d\cdot F^*\cdot\theta_Q\cdot F$ is nondegenerate, the projection $\mathrm{pr}_{2*}\cdot X$ of the solution X of the canonical equation of motion on $T^*Q \oplus TQ$ equals the differential equation X_2 with which we began, Eq. (3): we obtain no more[28] then we started with. (Note that this includes the second-order equation condition.)

VI. SUMMARY AND DISCUSSION

The fact that Newton's equations of motion are second-order differential equations has been shown to lead to a canonical form for the equivalent first-order equation of motion, a form that displays the features of the Hamiltonian formulation of mechanics even if a Lagrangian does not exist. Two requirements, the second-order equation condition and the demand for a single equation for the phase-velocity vector X_1, lead to a first-order equation that, without loss of generality, may be taken to involve differential forms on $T^*Q \oplus TQ$.

The dynamical trajectories on $T^*Q \oplus TQ$ are limited to a $2\times$ dim Q-dimensional subspace, and this restriction may be taken to be a consequence of the canonical first-order equation on $T^*Q \oplus TQ$. The canonical 2-form and the $p\cdot v$ term appear in the canonical first-order equation of motion as a result of this restriction and the second-order equation condition.

The relation between the phase velocity X_1 and the accelerations given by Newton's equations of motion is derived from the consistency condition that the velocity X_1 is tangent to the subspace of the dynamical trajectories. Indeed, this consistency condition alone leads to the canonical first-order equation of motion, as shown by the derivation of Eq. (45) in Sec. IVC.

[1]A. Lichnerowicz, in *Differential Geometrical Methods in Mathematical Physics, Bonn 1975*, edited by A. Dold and B. Eckmann (Springer-Verlag, New York, 1977), p. 377.

[2]A satisfying formulation of Newton's laws of motion is given in L. Eisenbud, Am. J. Phys. **26**, 144 (1958).

[3]See, e.g., P. J. Morrison and J. M. Greene, Phys. Rev. Lett. **45**, 790 (1980).

[4]The history of the early development of Hamiltonian mechanics is described in R. Dugas, *A History of Mechanics*, translated by J. R. Maddox (Routledge and Kegan Paul, London, 1957), and briefly in E. T. Whittaker, *A Treatise on the Analytical Dynamics of Particles and Rigid Bodies*, 4th ed. (Dover, New York, 1944), p. 264 and C. Lanczos, *The Variational Principles of Mechanics*, 4th ed. (University of Toronto, Toronto, 1970), p. 167.

[5]Here, canonical means having a standard form. Cf. the footnote on p. 342 of H. Goldstein, *Classical Mechanics*, 2nd ed. (Addison-Wesley, Reading, MA, 1980).

[6]A generalization of Hamilton's equations that is not based on the assumption of the existence of a potential energy function, but does assume a kinetic energy function, was given almost immediately after Hamilton published those equations—W. R. Hamilton, Report on the Fourth Meeting of the British Association for the Advancement of Science, Edinburgh, 1834, p. 513—by Jacobi; see Dugas, Ref. 4, p. 406.

[7]A. Sommerfeld, *Mechanics*, translated by M. O. Stern (Academic, New York, 1964).

[8]Goldstein's text described in Ref. 5.

[9]V. I. Arnold, *Mathematical Methods of Classical Mechanics*, translated by K. Vogtmann and A. Weinstein (Springer-Verlag, New York, 1978).

[10]R. Abraham and J. E. Marsden, *Foundations of Mechanics*, 2nd ed. (Benjamin/Cummings, Reading, MA, 1977).

[11]The differential geometry used here and in the following is described in Refs. 9 and 10. The notation, unless specifically introduced in the text, is that of Ref. 10 with the exceptions that the tangent map, denoted $T\phi$ there, is written ϕ_* here, the cotangent bundle is here designated π_Q: $T^*Q \rightarrow Q$, and $\langle p|v\rangle$ is used here to denote the evaluation of the covector p on the vector v.

[12]See pp. 213–215 of Ref. 10.

[13]This definition corresponds to the terminology of S. Sternberg, *Lectures on Differential Geometry* (Prentice-Hall, Englewood Cliffs, NJ, 1964), p. 166.

[14]Second-order differential equations can be defined without the second-order equation condition in terms of jet bundles [described, e.g., in K. Yana and S. Ishihara, *Tangent and Cotangent Bundles* (Dekker, New York, 1973)]. However, hiding that condition as in jet bundle theory would make the subsequent development less evident.

[15]Just as there are Lagrangians (e.g., $L = q$ on $Q = R$) that lead to inconsistent equations of motion, so there are Lagrangians that are inconsistent with the second-order equation condition. The example $L = (1 + y)\,v_x^2 - zx^2 - y$ on $Q = R^3$ was given in M. J. Gotay, Ph.D. thesis (University of Maryland, 1979).

[16]P. A. M. Dirac, Can. J. Math. **2**, 129 (1950); *Lectures on Quantum Mechanics* (Belfer Graduate School of Science Monograph Series #2, 1964); Proc. R. Soc. London Ser. A **246**, 326 (1958).

[17]The solution curve points of X_2 form a proper subset of TQ in generalized mechanics (see Ref. 16). This case is not considered here except for some remarks in the footnotes and in an example given in Sec. V in which X_2 is a solution of Lagrange's equations.

[18]The Whitney sum, described for example in D. Husemoller, *Fiber Bundles*

(McGraw-Hill, New York, 1966), is a type of product bundle of two vector bundles but here, as yet, M is not identified as a vector bundle. By the generalized Whitney sum is meant the space $M \oplus TQ = \{\tau_Q^{-1} \cdot q \times \mathrm{pr}^{-1} \cdot q$ for every $q \in Q\}$ with a manifold structure induced from those of M and TQ.

[19]R. Skinner, in *Abstracts of Contributed Papers for the Discussion Groups* (9th International Conference on General Relativity and Gravitation, Friedrich Schiller University, Jena, G. D. R., 1980), pp. 142–143.

[20]The notation in (17) denotes the diagonal map followed, in the case of the right-hand side, by $\sigma \cdot \phi \cdot \mathrm{pr}_1 \times \mathrm{pr}_2$, after which evaluation of the one-form on the vector is performed. This short-hand notation is used extensively in the rest of this paper.

[21]R. Jost, Rev. Mod. Phys. **36**, 572 (1964).

[22]J. L. Anderson and P. G. Bergmann, Phys. Rev. **83**, 1018 (1951).

[23]In the case of generalized mechanics, the map F should be chosen so that those acceleration components not determined by the equations of motion do not appear in (45).

[24]See p. 200 of Ref. 11.

[25]Finding such an L for a given X_2, i.e., for given forces, is called the inverse problem in Newtonian mechanics. The function L satisfying these conditions is not necessarily unique. Discussions of these matters, and references to earlier discussions, may be found in R. Cawley, J. Math. Phys. **21**, 2350 (1980); R. M. Santilli, *Foundations of Theoretical Mechanics I* (Springer-Verlag, New York, 1978); and N. A. Lemos, Phys. Rev. D **24**, 1036 (1981).

[26]This is not true if F is not a diffeomorphism, in which case part of the second-order equation condition is lost because of a degeneracy in $\bar{j}^* \cdot \omega_Q$: this lost part of the second-order equation condition must be imposed as an extra restriction on X_F.

[27]R. Skinner and R. Rusk, "Generalized Hamiltonian dynamics, I: formulation on $T^*Q \oplus TQ$", following paper.

[28]However, if F is not a diffeomorphism, we appear to obtain less since, in that case, $d \cdot F^* \cdot \theta_Q \cdot F$ is degenerate so the equation of motion on TQ may be satisfied if X_2 differs from $\mathrm{pr}_{2*} \cdot X$. This occurs, for instance, in degenerate-Lagrangian mechanics where the equation of motion determines X, and $\mathrm{pr}_{2*} \cdot X$, only up to a subspace.

Generalized Hamiltonian dynamics. I. Formulation on $T^*Q \oplus TQ$

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The Dirac–Bergmann generalized Hamiltonian dynamics for a degenerate-Lagrangian system is formulated on the Whitney sum $T^*Q \oplus TQ$ of the phase space T^*Q and the velocity space TQ over the configuration space Q. The formulation is related to those on T^*Q and TQ. Some ambiguities concerning generalized dynamics that have appeared in the literature are clarified.

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I. INTRODUCTION

The local Euler–Lagrange equations for a mechanical system in the configuration space Q,

$$\frac{d}{dt}\left[\frac{\partial L(q,\dot{q})}{\partial \dot{q}^i}\right] - \frac{\partial L(q,\dot{q})}{\partial q^i} = 0, \tag{1}$$

are[1] equivalent to a canonical first-order equation on the Whitney sum[2,3] $T^*Q \oplus TQ$ of phase space T^*Q and velocity space TQ. And this equivalence holds, unlike the situation for classical Hamiltonian mechanics, whether or not the Lagrangian is nondegenerate (hyperregular[4]). Therefore this canonical equation is suitable for discussions of generalized Hamiltonian dynamics,[5] the case that arises when locally the Hessian $\det[\partial^2 L(q,v)/\partial v^i \partial v^j]$ of the Lagrangian is zero so one cannot solve the canonical momenta-defining equations $p = \partial L/\partial v$ for every component $v^i = v^i(q,p)$ of the velocity.

Generalized dynamics is the finite-dimensional analog of gauge field theory, so the study of generalized dynamics is important for the light that it can throw on gauge theories. Indeed, Dirac[5] developed his form of generalized Hamiltonian dynamics for that reason.[6]

The study of generalized Hamiltonian dynamics began with pioneering works of Dirac[7] and, independently, Bergmann[8] and his collaborators, and has been translated into modern global mathematical language.[9–14] Nevertheless, some questions concerning this generalized dynamics, particularly regarding its gauge transformations, have remained unanswered or clouded in controversy.[15–21]

The global formulation of generalized Hamiltonian dynamics on $T^*Q \oplus TQ$ described below[22] appears simpler and more straightforward than previous formulations on velocity space TQ,[19,23] on phase space T^*Q, or its primary constraint submanifold, the presymplectic manifold (M, ω) of Ref. 13. The analog of the Hamiltonian on T^*Q involves arbitrary functions and requires solving the momenta-defining equations, while the closed 2-form ω on M, or that on TQ, is presymplectic with a degeneracy, determined by the momenta-defining equations, that may be different for different Lagrangians. On the other hand, the equivalent of the Hamiltonian in the present formulation of generalized Hamiltonian dynamics is well defined, one is not required to solve the momenta-defining equations for the velocities,[1] and the degeneracy in the corresponding 2-form is the same for all systems with motions in the same configuration space. As a result of this, ambiguities present in formulations on T^*Q or (M, ω) do not appear in the present formulation, as shown by a specific example in the Appendix. Furthermore, the relationship between the formulation of generalized dynamics on T^*Q and that on TQ is easily established from that on $T^*Q \oplus TQ$.

Kundt[24] has given a *local*[25] formulation on $T^*Q \oplus TQ$ of generalized dynamics, but his formulation has been subject to criticism.[13,14] Comparisons of Kundt's local formulation with the present global one are given in a few footnotes.

The canonical equation of motion determines the velocity vector on $T^*Q \oplus TQ$ only to within a vector subspace of $T(T^*Q \oplus TQ)$, so there are gauge transformations in generalized dynamics. These are discussed in the following paper.[26]

The canonical equation of motion on $T^*Q \oplus TQ$, which is equivalent to the Euler–Lagrange equations on Q, and the primary constraint submanifold, which results from the degeneracy of the canonical 2-form, are described in Sec. II. The final constraint submanifold, the submanifold on which the motions take place, is derived in Sec. III by three methods: by the Gotay–Nester–Hinds algorithm[13,14] in Sec. IIIA, by a technique that gives results useful for the later discussion of gauge transformations in Sec. IIIB, and by the original method of Dirac[5] in Sec. IIIC.

The formulation on T^*Q of generalized dynamics is given in Sec. IV, which contains a discussion in Subsec. A of what corresponds to the equation of motion on T^*Q, the determination in Subsec. B of the final constraint submanifold in T^*Q and the relationship to the corresponding submanifold in $T^*Q \oplus TQ$. A similar development of the dynamics on TQ is presented in Sec. V, with corresponding Subsecs. A and B. The relationship between the formulations on $T^*Q \oplus TQ$, T^*Q, and TQ is discussed in Subsec. C.

A short summary and discussion of the present work is given in Sec. VI. An example of those generalized dynamical systems that have been the subject of controversy in the literature is worked out within the formulation on $T^*Q \oplus TQ$ in an Appendix.

II. THE CANONICAL EQUATION OF MOTION[1]

Consider a mechanical system whose dynamical behavior on configuration space Q is described by the Lagrangian $L: TQ \to R$. The Euler–Lagrange equations for the system are

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equivalent to the canonical first-order equation of motion, described below, that generalizes the Hamiltonian formulation.

The canonical equation involves a differential 1-form on the Whitney sum $W_0 = T^*Q \oplus TQ$, with canonical projection pr_i $(i = 1, 2)$ on the ith factor. There are natural bundle coordinates on W_0 induced by the coordinate functions q_Q^i on a chart about q_Q in Q:

$$q^i = q_Q^i \cdot \pi_Q \cdot \mathrm{pr}_1, p_i = \langle \mathrm{pr}_1 | \partial / \partial q_Q^i \rangle$$

and

$$v^i = \langle dq_Q^i | \mathrm{pr}_2 \rangle. \tag{2}$$

The *inertial 1-form* of the canonical equation contains the pullback[27] from T^*Q, $\omega = \mathrm{pr}_1^* \cdot \omega_Q$, of the canonical 2-form ω_Q on T^*Q with

$$\omega_Q = -d\theta_Q \quad \text{and} \quad \theta_Q = \pi_Q^*: T^*Q \to T^*T^*Q. \tag{3}$$

The *dynamical 1-form* of the equation of motion is determined by the *dynamical function* (corresponding to the Hamiltonian)

$$D: W_0 \to R: w \mapsto \langle \mathrm{pr}_1 \cdot w | \mathrm{pr}_2 \cdot w \rangle - L \cdot \mathrm{pr}_2 \cdot w. \tag{4}$$

Since the Lagrangian is degenerate, there is no Legendre transformation that transforms the dynamical function on $T^*Q \oplus TQ$ to a Hamiltonian on T^*Q.

The equation of motion determines a vector field X, an extended velocity vector, on the subspace S consisting of those points of W_0 on which solutions, tangent to S, of the canonical equation exist:

$$X: S \subset W_0 \to TS \subset TW_0. \tag{5}$$

The subspace S is called the *final constraint submanifold*.

The *canonical first-order equation of motion* for an extended velocity vector X is

$$i(X) \cdot \omega = dD. \tag{6}$$

A consistent solution X satisfies this equation of motion and is tangent to the solution submanifold S. This *consistency condition* is required in order that the motions derived from X do not lead into regions in which it is not possible to satisfy the equation of motion.

The canonical equation of motion cannot be solved at every point of $T^*Q \oplus TQ$ because of the properties of ω and D. Indeed, since for each vector Y in

$$TW_0^{\perp} = \{ Z \in TW_0 \text{ such that } \mathrm{pr}_{1*} \cdot Z = 0 \}, \tag{7}$$

$i(Y) \cdot \omega = 0$, the equation of motion cannot be solved at $w = \tau_{W_0} \cdot Y$ unless $i(Y) \cdot dD |_w = 0$. Therefore the canonical equation of motion can be solved only at points w in W_0 for which the map $\mathrm{pr}_1 - \mathbf{F}L \cdot \mathrm{pr}_2$ gives zero: here $\mathbf{F}L: TQ \to T^*Q$ is the fiber derivative of L, which satisfies $\pi_Q \cdot \mathbf{F}L = \tau_Q$. These points form the *primary constraint submanifold*

$$\begin{aligned} W_1 = \{ w \in W_0 \quad &\text{such that} \quad i(Y) \cdot dD |_w \\ = 0 \quad &\text{for every } Y \text{ in } TW_0^{\perp} |_w \} = \text{graph } \mathbf{F}L. \end{aligned} \tag{8}$$

Where no confusion with other inclusion maps can arise, an inclusion map is designated here by j_{domain}, as in $j_{W_1}: W_1 \to W_0$. Also, it is assumed here that the fiber derivative is smooth so the canonical map

$$\overline{\mathbf{F}L}: TQ \to \text{graph } \mathbf{F}L \tag{9}$$

is a diffeomorphism, with

$$\mathrm{pr}_2 \cdot j_{W_1} = (\overline{\mathbf{F}L})^{-1} \quad \text{and} \quad \mathrm{pr}_1 \cdot j_{W_1} \cdot \overline{\mathbf{F}L} = \mathbf{F}L. \tag{10}$$

For the problems of interest here, the Lagrangian L is degenerate so, in natural bundle coordinates, $\det(\partial^2 L / \partial v^i \partial v^j) = 0$. Therefore there exist vectors in $TW_0^{\perp}$, having local coordinate representations of the form $a^i \partial / \partial v^i$, that annul $\partial L / \partial v^j$ and, of course, p_j. These vectors are tangent to W_1 and thus lie in and, indeed, span $TW_0^{\perp} \cap \underline{TW}_1$; for any inclusion j of any manifold W in W_0, $\underline{TW}$ is defined by $\underline{TW} = j_* \cdot TW$. We assume that $m = \dim(TW_0^{\perp} \cap \underline{TW}_1)$ is constant over W_1.

The canonical equation and the consistency condition do not, in general, determine a unique X if the Lagrangian is degenerate: if X is one consistent solution on S of the equation of motion, then so is $X + Y$ for any $Y \in TW_0^{\perp} \cap \underline{TS}$. Thus in general, a general consistent solution is not a true vector field being determined only to within a vector subspace of $TW_0^{\perp}$. Dirac[5] has introduced the adjective *generalized* to describe such systems.

III. FINAL CONSTRAINT SUBMANIFOLD

For a degenerate-Lagrangian system, it is not possible to satisfy the canonical equation of motion and the consistency condition at all points of W_1. The final constraint submanifold S can be calculated through use of any of the following three algorithms.

This submanifold S is the unique maximal submanifold[13] upon which the equation of motion has consistent solutions. (The equation of motion, as noted before, also has solutions that are not tangent to S.)

Each vector $Y_1 \in \mathrm{pr}_{1*} \cdot \underline{TS}$ corresponds on a one-to-one basis to an element $Y \in \underline{TS} / (TW_0^{\perp} \cap \underline{TS})$ by $\mathrm{pr}_{1*} \cdot Y' = Y_1$, where Y' is a typical element in $\underline{TS}$ representing Y. Also, $\mathrm{pr}_{1*} \cdot X$ is uniquely determined by the canonical equation of motion since ω_Q is nondegenerate. Thus the equation of motion determines a unique element $X \in \underline{TS} / (TW_0^{\perp} \cap TS)$.

A. Gotay–Nester–Hinds algorithm[13]

Let W_l be a submanifold of W_0, with inclusion j_l, and define $\underline{W}_l \subset W_0$ by $\underline{W}_l = j_l \cdot W_l$. The *sympletic complement* $TW_l^{\perp}$ of $\underline{TW}_l$ in TW_0 for $l \geqslant 0$ is defined by

$$\begin{aligned} TW_l^{\perp} &= \{ Y \in TW_0 \quad \text{such that} \quad \omega(Z, Y)|_{\underline{W}_l} \\ &= 0 \quad \text{for every} \quad Z \in \underline{TW}_l \} \\ &= \{ Y \in TW_0 \quad \text{such that} \quad j_l^* \cdot i(Y) \cdot \omega = 0 \}. \end{aligned} \tag{11}$$

The Gotay–Nester–Hinds algorithm applied to the present problem generates a sequence of submanifolds $\{ W_l \}$, with $j_{W_l}: W_l \to W_{l-1}$, defined by[28]

$$W_{l+1} = \{ w \in \underline{W}_l \quad \text{such that} \quad \langle dD | TW_l^{\perp} \rangle (w) = 0 \}, \tag{12}$$

with $j_l = j_{W_1} \cdot j_{W_2} \cdot \cdots \cdot j_{W_l}$. We assume that there exists a K such that $W_K = W_{K+1}$ is a submanifold of W_0. This W_K is the final constraint submanifold S.

There are other ways to generate the final constraint submanifold, the following in Subsec. B being useful for discussing gauge transformations[26] and the one in Subsec. C being closer to the spirit of Dirac's original paper[5] on the subject.

B. Algorithm useful in describing gauge transformations

Since $TW_j^{\perp}$ consists of vectors Y in TW_0 that satisfy $j_j^* \cdot i(Y) \cdot \omega = 0$, $i(Y) \cdot \omega$ can be written locally in terms of a complete set $\{\phi^{\alpha j}; \alpha = 1, 2, ..., \dim W_0 - \dim W_j\}$ of constraint functions for W_j as (with summation assumed over repeated alphabetic indices) $i(Y) \cdot \omega = a_\alpha d\phi^{\alpha j}$ for some $a_\alpha : W_0 \to R$. This observation provides the basis for the following algorithm that determines local forms for the constraints. We start with $TW_0^{\perp}$ and W_0.

The algorithm proceeds as follows. Given, for $j \geqslant 0$, W_j and $TW_j^{\perp}$, spanned by the local vector fields $\{Y^{\alpha j+1}\}$, find W_{j+1} as determined by the constraints[11] $\{\langle dD \mid Y^{\alpha j+1}\rangle\}$. It may happen that some of these constraints, or a linear combination of them, have a vanishing differential on W_{j+1}, but it is the points of W_{j+1} that are of concern, not the form of the constraint.[29] Replace any constraint $\langle dD \mid Y^{\alpha'' j}\rangle$, or linear combination of those, whose differential vanishes by an equivalent constraint function $\phi^{\alpha'' j}$ whose differential remains finite and does not vanish on W_j. Find a maximal set of functions $\{a_\alpha\} = \{a_{\alpha'}, a_{\alpha''}\}$ on W_{j+1} for which

$$i(TW_0^{\perp}) \cdot (a_{\alpha'} d\langle dD \mid Y^{\alpha' j}\rangle + a_{\alpha''} d\phi^{\alpha'' j}) = 0. \qquad (13)$$

Then solve, on W_{j+1},

$$i(Y) \cdot \omega = d(\langle dD \mid a_{\alpha'} Y^{\alpha' j}\rangle + a_{\alpha''} \phi^{\alpha'' j}) \qquad (14)$$

for a maximal set of linearly independent Y's that span $TW_{j+1}^{\perp}$. [The condition (13) is the necessary and sufficient condition that Eq. (14) has a solution.] The procedure stops at $j+1$ equal to that $K+1$ that satisfies $W_K = W_{K+1}$.

C. Dirac's algorithm[5]

The constraint functions can be derived in another way that is similar to that used by Dirac in his original paper. This method is based on the observation that on W_j, $i(X^j) \cdot \omega = dD$ has, by a theorem due to Gotay, Nester, and Hinds,[13] a solution X^j tangent to W_{j-1} since $\langle dD \mid TW_{j-1}^{\perp}\rangle|_{W_j} = 0$. Then on W_j, for a's that satisfy (13),

$$\langle dD \mid Y^{\alpha j}\rangle = -\mathbf{L}_{X^j} \cdot (a_{\alpha'}^{\alpha j} \langle dD \mid Y^{\alpha' j-1}\rangle + a_{\alpha''}^{\alpha j} \phi^{\alpha'' j-1}). \qquad (15)$$

The condition (13) is equivalent to requiring that the local function in parentheses is independent, to first order, of the velocity coordinates v^i. The Lie derivative $\mathbf{L}_{X^j}$ is in this case the time derivative since

$$(X^{j+1} - X^j)|_{W_{j+1}} \in TW_0^{\perp} \cap \underline{TW_{j-1}}|_{W_{j+1}}, \qquad (16)$$

and X^j is determined only to elements in $TW_0^{\perp} \cap \underline{TW_{j-1}}$. Also the Lie derivative, with respect to such elements, of the function in parentheses in (15) is zero. Thus the set of constraint functions for W_{j+1} is given, in essence, by requiring that the time derivatives of the complete set of constraint functions (with nonvanishing differentials) for W_j be zero.[30]

Dirac's algorithm determines locally the final constraint submanifold as follows: On W_j, determine $X^j \in \underline{TW_{j-1}}$ from $i(X_j) \cdot \omega = dD$. (Note that X^j for $j > 1$ is obtained easily from X^1.) Find all possible linear combinations of the constraints for W_j whose differentials are finite and not zero and are independent of dv^i. Set equal to zero the time derivatives, as calculated with $\mathbf{L}_{X_j}$, of these combinations to get W_{j+1}. Proceed until $j+1$ equals that $K+1$ for which $W_K = W_{K+1}$.

IV. THE DYNAMICS ON T^*Q

To discuss the dynamics on T^*Q, we introduce the submanifolds $M_1 = \operatorname{Im} FL$, the base space for the bundle $r_1 : W_1 \to M_1$ with $\mathrm{pr}_1 \cdot j_{W_1} = j_{M_1} \cdot r_1$ and, for $i = 1, 2, ..., K$,

$$M_i = \{m \in M_0 \quad \text{such that } m = r_1 \cdot j_{W_2} \cdot \cdots \cdot j_{W_i} \cdot w_i \text{ for every } w_i \text{ in } W_i\} \subset T^*Q = M_0. \qquad (17)$$

This yields the maps $r_i = r_1|_{W_i}$ and $j_{M_i} : M_i \to M_{i-1}$, with $r_{i-1} \cdot j_{W_i} = j_{M_i} \cdot r_i$.

A. Equation of motion on T^*Q

A consistent solution to the canonical equation of motion $X \in \underline{TS}$ can be projected to TT^*Q by the tangent of pr_1. Since $\mathrm{pr}_{1*} \cdot TW_0^{\perp} = 0$, the indeterminacy in X does not result in any uncertainty in $\mathrm{pr}_{1*} \cdot X$. In the nondegenerate case, the equation of motion on T^*Q is the 1-form equation that $\mathrm{pr}_{1*} \cdot X$ satisfies. However, matters are more complicated in the degenerate case.

The inertial 1-form $i(X) \cdot \omega$ involves, everywhere on $T^*Q \oplus TQ$, only the $\mathrm{pr}_{1*} \cdot X$ part of any vector field X. However, only on $\underline{W}_1$ is it possible for the inertial 1-form to equal the dynamical 1-form dD. This suggests that an equation of motion on the final constraint submanifold of T^*Q might be found by solving

$$[\mathrm{pr}_1^* \cdot i(\mathrm{pr}_{1*} \cdot X) \cdot \omega_Q \cdot \mathrm{pr}_1 - dD]|_{\underline{W}_1} = 0 \qquad (18)$$

for the unique solution $\mathrm{pr}_{1*} \cdot X$ and substituting that into $i(\mathrm{pr}_{1*} \cdot X) \cdot \omega_Q$ to determine the dynamical 1-form on that portion of T^*Q. The problem with this procedure in the degenerate-Lagrangian case is that $\mathrm{pr}_{1*} \cdot X(w)$ is not equal to $\mathrm{pr}_{1*} \cdot X(w')$ for every w and w' in $\underline{W}_1$ such that $\mathrm{pr}_1 \cdot w = \mathrm{pr}_1 \cdot w'$. Thus $i(\mathrm{pr}_{1*} \cdot X) \cdot \omega_Q$ is not a 1-form: $T^*Q \to T^*T^*Q$.

This result can be seen also by looking at the dynamical 1-form dD on $\underline{W}_1$: Since, for w on $\underline{W}_1$, $\langle dD \mid Y\rangle(w)$ is linear and homogeneous in $\mathrm{pr}_{1*} \cdot Y$,

$$\langle dD \mid Y\rangle|_w = \langle \beta^w | \mathrm{pr}_{1*} \cdot Y\rangle|_{\mathrm{pr}_1 \cdot w} \qquad (19)$$

defines an element $\beta^w \in T^*_{\mathrm{pr}_1 \cdot w} T^*Q$. However, β^w and $\beta^{w'}$ are not equal for every w and w' satisfying $\mathrm{pr} \cdot w = \mathrm{pr} \cdot w'$.

To see how $\mathrm{pr}_{1*} \cdot X$ varies along the fibers of $r_1 : W_1 \to M_1$, select any two points on one fiber, join them with a curve generated by a vector field $Y : \underline{W}_1 \to TW_0^{\perp} \cap \underline{TW}_1$, evaluate X at the two points, project down to TT^*Q, and take the differences at the two points. In the appropriate limit, we see that if X is a solution of $[i(X) \cdot \omega - dD]_{\underline{W}_1} = 0$, we can write

$$0 = [i(\mathbf{L}_Y X) \cdot \omega - d\langle dD \mid Y\rangle]|_{\underline{W}_1}. \qquad (20)$$

Since $\langle dD \mid Y\rangle$ is a constraint function for W_1, $\mathbf{L}_Y \cdot X \in TW_1^{\perp}$ so $\mathrm{pr}_{1*} \cdot \mathbf{L}_Y X \in \mathrm{pr}_{1*} \cdot TW_1^{\perp}$. For $Z \in TW_1^{\perp}$, we have

$$0 = j_{W_1 *} \cdot i(Z) \cdot \omega = r_{1*} \cdot [\, j_{M_1 *} \cdot i(\mathrm{pr}_{1*} \cdot Z) \cdot \omega_Q \,]. \quad (21)$$

Therefore $\mathrm{pr}_{1*} \cdot Z \in TM_1^{\perp}$ where, for M_l a submanifold of T^*Q with inclusion $h_l = j_{M_1} \cdot j_{M_2} \cdot \cdots \cdot j_{M_l}$,

$$TM_l^{\perp} = \{\, Y_1 \in T^*Q \quad \text{such that} \quad h_l^* \cdot i(Y_1) \cdot \omega_Q = 0 \,\}. \quad (22)$$

We conclude that $\mathrm{pr}_{1*} \cdot \mathrm{L}_Y X \in TM_1^{\perp}$. Since, for $p = \mathrm{pr}_1 \cdot w = \mathrm{pr}_1 \cdot w'$, $T_p M_1^{\perp}$ is a vector space, and the rate of change of X at each point along the curve lies in $T_p M_1^{\perp}$, the difference $\mathrm{pr}_{1*} \cdot X(w) - \mathrm{pr}_{1*} \cdot X(w')$ lies in $TM_1^{\perp}$. Thus $X_1 = \mathrm{pr}_{1*} \cdot X$ is determined at the point p only modulo elements in $TM_1^{\perp}$.

To obtain a typical element X_1, we assume a local section

$$\sigma: U \subset T^*Q \to T^*Q \oplus TQ \quad (23)$$

that on $U \cap M_1$ picks out one point on each fiber of $r_1: W_1 \to M_1$. We set

$$dD = d(D \cdot \sigma \cdot \mathrm{pr}_1) + d(D - D \cdot \sigma \cdot \mathrm{pr}_1), \quad (24)$$

and note that $d(D - D \cdot \sigma \cdot \mathrm{pr}_1)$ corresponds[31] to the difference between $\mathrm{pr}_{1*} \cdot X$ at two different points on the same fiber so is equal to the differential of a constraint for W_1. Therefore we get a typical element X_1 from the vanishing of

$$\mathrm{pr}_1^* [\, i(X_1) \cdot \omega_Q - d(D \cdot \sigma) \,], \quad (25)$$

or, alternatively by taking the pullback by σ^* of this,

$$i(X_1) \cdot \omega_Q - dH, \quad (26)$$

where H is the "Hamiltonian"

$$H = D \cdot \sigma: U \subset T^*Q \to R. \quad (27)$$

The resulting equation of motion determines $\mathrm{pr}_{1*} \cdot X$ up to elements in $TM_1^{\perp}$. Thus one could obtain an equation of motion for all $\mathrm{pr}_{1*} \cdot X$ by adding to dH arbitrary linear combinations of the differentials of all the constraint functions for M_1 in T^*Q, this being the procedure followed by Dirac.[5,7]

Alternatively, we could work on M_1 alone and take the equation of motion on M_1 to be the pullback by $j_{M_1}^*$ of (26). Since X_1 must be tangent to M_1, this is equivalent, with $X_1 = j_{M_1 *} \cdot X_{M_1}$, to

$$i(X_{M_1}) \cdot j_{M_1}^* \cdot \omega_Q = d(H \cdot j_{M_1}), \quad (28)$$

the equation of motion with which Gotay, Nester, and Hinds[13] started their discussion of Dirac's generalized mechanics.

B. The Gotay–Nester–Hinds algorithm on T^*Q

We now show that the algorithm generates the sequence

$$M_K \xrightarrow[j_{M_K}]{} \cdots M_2 \xrightarrow[j_{M_2}]{} M_1 \xrightarrow[j_{M_1}]{} M_0 = T^*Q. \quad (29)$$

The map h_l satisfies $\mathrm{pr}_1 \cdot j_l = h_l \cdot r_l$ so, if Y in $TW_0|_W$ lies in $TW_l^{\perp}$, then

$$h_l^* \cdot i(\mathrm{pr}_{1*} \cdot Y) \cdot \omega_Q = 0. \quad (30)$$

Therefore pointwise,

$$TM_l^{\perp} = \mathrm{pr}_{1*} \cdot TW_l^{\perp}. \quad (31)$$

Finally, pointwise,

$$\langle dH \,|\, TM_l^{\perp} \rangle|_{h_l \cdot r_l \cdot W_l} = \langle dD \,|\, \sigma_* \cdot \mathrm{pr}_{1*} \cdot TW_l^{\perp} \rangle|_{\sigma \cdot h_l \cdot r_l \cdot W_l}. \quad (32)$$

However, if Y lies in $TW_l^{\perp}$, then $j_l^* \cdot i(\sigma_* \cdot \mathrm{pr}_{1*} \cdot Y) \cdot \omega$ is zero and thus $\sigma_* \cdot \mathrm{pr}_{1*} \cdot Y$ lies in $TW_l^{\perp}$. Therefore $r_{l+1} \cdot W_{l+1}$ is the set

$$M_{l+1} = \{ p \in T^*Q \quad \text{such that} \quad \langle dH \,|\, TM_l^{\perp} \rangle (p) = 0 \}. \quad (33)$$

V. THE DYNAMICS ON TQ

A. The equation of motion on TQ

The equation of motion on $T^*Q \oplus TQ$ has been shown[1] to be equivalent to its pullback, by $j_{W_1}^*$, to an equation of motion on W_1; all that is lost by the pullback is the set of constraints for W_1 and part of the second-order equation condition (lost because of the degeneracy of ω_L defined below). The pulled-back equation and imposition of the lost part of the second-order equation condition is equivalent, by the diffeomorphism $\overline{\mathbf{FL}}^{-1}$, to a second-order equation on Q.

Since a consistent solution X to the equation of motion, where it exists, is tangent to W_1, $X = j_{W_1 *} \cdot X_{W_1}$, we have that $X_2 = \mathrm{pr}_{2*} \cdot X$ determines $X = j_{W_1 *} \cdot \overline{\mathbf{FL}_*} \cdot X_2$. The arbitrariness in X is preserved since, if Z in $TW_0^{\perp}$ is not zero, neither is $Z_2 = \mathrm{pr}_{2*} \cdot Z$.

The motion 1-form pulls back to TQ with $(j_{W_1} \cdot \overline{\mathbf{FL}})^*$. The energy is defined by $E = D \cdot j_{W_1} \cdot \overline{\mathbf{FL}}$ and we set $\omega_L = \mathbf{FL}^* \cdot \omega_Q$ to obtain the motion 1-form on TQ

$$i(X_2) \cdot \omega_L - dE. \quad (34)$$

The vector X_2 is determined (up to some vectors in $TW_0^{\perp}$) by the vanishing of this 1-form and the second-order equation condition

$$\tau_{Q*} \cdot X_2 = id_{TQ}, \quad (35)$$

plus the consistency condition that X_2 be tangent to the final constraint submanifold.

B. The Gotay–Nester–Hinds algorithm on TQ[32]

The algorithm generates the sequence of submanifolds

$$\cdots \to \mathrm{N}_3 \xrightarrow[j_{N_3}]{} N_2 \xrightarrow[j_{N_2}]{} N_1 = TQ. \quad (36)$$

We define, with $j_{N_1} = id_{TQ}$,

$$g_l = j_{N_1} \cdot j_{N_2} \cdot \cdots \cdot j_{N_l}. \quad (37)$$

For $Y_{W_1} = \overline{\mathbf{FL}}_* \cdot Y_2$, we have that

$$g_l^* \cdot i(Y_2) \cdot \omega_L = g_l^* \cdot \overline{\mathbf{FL}}^* \cdot j_{W_1}^* \cdot i(j_{W_1 *} \cdot Y_{W_1}) \cdot \omega. \quad (38)$$

Since $\overline{\mathbf{FL}}$ is a diffeomorphism, we have, for $l = 1$, that $Y_2 \in TN_l^{\perp}$ iff $j_{W_1 *} \cdot \overline{\mathbf{FL}}_* \cdot Y_2$ lies in $TW_1^{\perp}$. Assume that pointwise $j_{W_1 *} \cdot \overline{\mathbf{FL}}_* \cdot TN_l^{\perp} = TW_l^{\perp}$ is true for one value of l. Then

$$\langle dE \,|\, TN_l^{\perp} \rangle (n) = \langle dD \,|\, TW_l^{\perp} \rangle (j_{W_1} \cdot \overline{\mathbf{FL}} \cdot n), \quad (39)$$

so $n \in N_{l+1}$ iff $j_{W_1} \cdot \overline{\mathbf{FL}} \cdot n$ lies in W_{l+1}. Thus we have, pointwise, $W_{l+1} = j_{W_1} \cdot \overline{\mathbf{FL}} \cdot N_{l+1}$ or N_{l+1}

$= \mathrm{pr}_2 \cdot W_{l+1}$. Therefore $j_{W_1} \cdot \overline{\mathbf{FL}} \cdot g_{l+1} \cdot (\mathrm{pr}_2|_{W_{l+1}}) = j_{l+1}$ so, by (38), $TN_{l+1}^{\perp} = \mathrm{pr}_{2*} \cdot TW_{l+1}^{\perp}$, pointwise. Thus by induction, $N_j = \mathrm{pr}_2 \cdot W_j$ pointwise for each j.

C. Relationships between the formulations on phase space, velocity space, and their Whitney sum[33]

Formulas expressing the relationships between the different elements of generalized mechanics—velocity vectors, inertial 2-forms, and generating functions (dynamical function, "Hamiltonian," energy)—are given above or follow from $(\mathrm{pr}_1 - \mathbf{FL} \cdot \mathrm{pr}_2)|_{W_1} = 0$ as well as its consequences, such as the tangent of that map restricted to TW_1. Complications in these relationships arise because of local gauge invariances[26] or, equivalently, because the velocity vectors on the Whitney sum, velocity space, and phase space are determined only up to elements in a vector space, $V_{2\,\tan} = TW_0^{\perp} \cap \underline{TS}$, $\mathrm{pr}_{2*} \cdot V_{2\,\tan}$, and $TM_1^{\perp} \cap \mathrm{pr}_{1*} \cdot \underline{TS}$ respectively.

A velocity vector X on the Whitney sum projects down, by pr_{2*}, to a velocity vector X_2 on TQ, preserving its indeterminacy, and can be regained by use of $\mathrm{pr}_2 \cdot j_{W_1} = (\overline{\mathbf{FL}})^{-1}$. On the other hand, a velocity vector X_1 on phase space is not obtained by the projection pr_{1*}, but rather by choosing a local section σ (23) and relating X_1 to $X|_\sigma$. The difference between the X_1's corresponding to two local sections lies in $TM_1^{\perp}$. These relations result from the fact that the primary constraint submanifold W_1 is related to TQ by the diffeomorphism $\overline{\mathbf{FL}}$ and to M_1, a proper submanifold of T^*Q, by the bundle map r_1.

The velocity vector X on the Whitney sum satisfies the second-order equation condition, unless the Lagrangian is inconsistent with that, so $\mathrm{pr}_{2*} \cdot X$ and X_1 do too. However, the equation of motion on TQ involves the degenerate ω_L and may possess[23] consistent solutions X_2' that do not satisfy the second-order equation condition; nevertheless, if there is a consistent solution, which satisfies the second-order equation condition, on $T^*Q \oplus TQ$, there is a consistent solution on TQ that satisfies that condition, namely $X_2 = \mathrm{pr}_{2*} \cdot X$.

One can, in this way, relate the formulations on T^*Q and TQ through the "master" formulation on $T^*Q \oplus TQ$, which contains them both. And since the velocity vector on $T^*Q \oplus TQ$ determines motions that satisfy[1] the Euler–Lagrange equations for the Lagrangian L, there are solutions X_1 and X_2 on T^*Q and TQ, respectively, that do too.

VI. SUMMARY AND DISCUSSION

The canonical equation of motion on the Whitney sum $T^*Q \oplus TQ$ of phase space and velocity space is equivalent to the Euler–Lagrange equations even in generalized dynamics and "spreads" them out[1] into the second-order equation condition, the definition of the map $\mathbf{FL}$, an equation for the momenta velocities $\dot{p}_i$ and, through a consistency condition, an equation for the accelerations $\dot{v}^i$. The formulation of generalized Hamiltonian dynamics on $T^*Q \oplus TQ$ does not require one to solve the momenta-defining equations $p = \partial L / \partial v$, as is necessary for the formulation on T^*Q (and leading in some cases to problems, as shown by the example[16] given in the Appendix), nor to eliminate those solutions that do not satisfy the second-order equation condition, as is necessary[23] on TQ.

The problems in generalized mechanics are that the motions are restricted by constraints and that the trajectories are not unique. The constraints can be calculated by means of the Gotay–Nester–Hinds algorithm[13] or others. The procedure on $T^*Q \oplus TQ$ is straightforward, as shown by an example in the Appendix. The indeterminacy in the extended velocity vector $X(w)$ due to the degeneracy of ω lies in $T_w W_0^{\perp}$, a vector surface of $T_w W_0$ that does not depend on the Lagrangian, whereas those for $X_2(v)$ and $X_1(p)$, on $T_v Q$ and $T_p^* Q$, respectively, do depend on L. The gauge transformations that relate the different possible trajectories are discussed, on the basis of the formulation on $T^*Q \oplus TQ$, in the following paper,[26] which provides a straightforward resolution of the gauge problems discussed in the literature.

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APPENDIX

The final constraint submanifold and the solution X of the canonical equation of motion are calculated, and briefly discussed, for a typical case[16] of those generalized mechanical Lagrangians that have sparked controversy in the literature.

The calculation is presented in abbreviated form, beginning with the Lagrangian, the constraint submanifolds given by the constraint equations required beyond those given above that, vectors spanning the symplectic complement given in the same way, a general vector T in $TS^{\perp} \cap \underline{TS}$ with small Greek letters representing arbitrary constants, and the time-dependent consistent solution X with capital Latin letters representing arbitrary functions:

$$L = v_x v_z^2 + \tfrac{1}{2} y z^2,$$

$$W_0 = \{x, y, z, p_x, p_y, p_z, v_x, v_y, v_z\},$$

$$TW_0^{\perp}: \frac{\partial}{\partial v_x}, \frac{\partial}{\partial v_y}, \frac{\partial}{\partial v_z},$$

$$W_1: p_x - v_z^2 = 0, p_y = 0, \quad p_z - 2 v_x v_z = 0,$$

$$TW_1^{\perp}: \frac{\partial}{\partial y},$$

$$W_2: z = 0, \quad TW_2^{\perp}: \frac{\partial}{\partial p_z},$$

$$W_3: v_z = 0, \quad \text{so} \quad p_x = 0, p_z = 0,$$

$$TW_3^{\perp}: \frac{\partial}{\partial x}, \frac{\partial}{\partial z},$$

$$T = \alpha \frac{\partial}{\partial v_x} + \beta \frac{\partial}{\partial x} + \gamma \frac{\partial}{\partial v_y} + \delta \frac{\partial}{\partial y},$$

$$X = A \frac{\partial}{\partial v_x} + B \frac{\partial}{\partial v_y} + v_x \frac{\partial}{\partial x} + v_y \frac{\partial}{\partial y}.$$

Frenkel missed the constraint p_z: this constraint follows in the formulation on T^*Q from the equation of motion

$\dot{x} = p_z/(2p_x^{1/2})$ and the constraint p_x. One must examine all the component equations of motion to see that they are consistent on the final constraint submanifold. The reason that, working on T^*Q, one has to examine all components of the equation of motion is that solving the momenta-defining equations, not required on $T^*Q \oplus TQ$, may hide some constraints, as it does in this case and in an example [his Eq. (1)] due to Cawley.[17]

The vector $\partial/\partial z$ corresponding to the constraint p_z is not tangent to $\underline{S}$, nor is the vector $\partial/\partial p_z$ corresponding to the constraint z, so these vectors do not appear in T. In the terminology of Dirac,[5,7] z and p_z are second-class constraints.

Cawley[17] claims that the constraint p_z would be missed without an "augmented algorithm" and a similar claim, but with a different algorithm, has been made by Di Stefano.[21] However, there is no ambiguity about these constraints, and no need to formulate any augmented algorithm in the formulation of generalized dynamics on $T^*Q \oplus TQ$, and none on T^*Q if one imposes the necessary requirement of the consistency of all components of the equation of motion.

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Generalized Hamiltonian dynamics. II. Gauge transformations

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Generalized Hamiltonian dynamics is the finite-dimensional version of gauge field theory and possesses invariance properties corresponding to gauge invariances. It is argued herein that a proper description of the finite-dimensional gauge transformations requires a time-dependent formalism. With this, local and global gauge transformations can be distinguished, and the insight obtained from this distinction clarifies some ambiguities that have appeared in the literature. In particular, the time-dependent formalism provides a precise statement for Dirac's conjecture concerning the form of the generalized Hamiltonian on phase space.

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I. INTRODUCTION

Generalized Hamiltonian dynamics is the mechanics of a discrete system in a finite-dimensional space Q whose motions are described by a degenerate Lagrangian L, one for which the momenta-defining equations $p = \partial L/\partial v$ cannot be solved for every component $v^i(q,p)$ of the velocity. Each of the various forms of the equation of motion[1] on T^*Q, TQ, or their Whitney sum[2,3] $T^*Q \oplus TQ$ possesses consistent solutions only over a proper submanifold of the base space and, in general, does not determine a single vector field (the relevant "velocity" vector). Rather, each determines a subset of the tangent space over each point of the final constraint submanifold in the base space T^*Q, TQ, or $T^*Q \oplus TQ$. A consistent solution of the equation of motion is a smooth vector field on the final constraint submanifold with values in those subsets, and the difference between two consistent solutions has values in a vector subspace over each point. Furthermore, consistent solutions are physically indistinguishable, so that transformations that map one consistent solution into another are called gauge transformations.

The gauge transformations of generalized Hamiltonian dynamics have been the subject of controversy in the literature.[4-13] The study of gauge transformations given below shows the origin of that controversy and eliminates the ambiguities present in the literature. It is argued below that a time-dependent formulation of generalized Hamiltonian dynamics is necessary for the definition of and discussions on gauge transformations. The time-dependent formalism displays clearly the difference between global and local gauge transformations, the former involving arbitrary constants, the latter arbitrary time-dependent functions. Some of the controversy in the literature results from the failure of the time-independent formulation to display that difference clearly.

A brief outline of the formulation on $T^*Q \oplus TQ$ of generalized Hamiltonian dynamics is given in Sec. II. The argument for the need to describe gauge transformations within a time-dependent formalism and that formalism itself are presented in Sec. III. The definition of gauge transformations and the general properties of their generators appear in Sec. IV. The relationship between the generators of gauge transformations and first class constraints is the topic of Sec. V. An important class of such generators is derived in Sec. VI, where the distinction between global and local gauge transformations appears. Dirac's conjecture,[14] the subject of much of the controversy in the literature, is discussed and clarified in Sec. VII. The gauge transformations for the formulations of generalized dynamics on phase space T^*Q and velocity space TQ are given in Sec. VIII in terms of the formulation on $T^*Q \oplus TQ$. A brief summary and conclusions are given in Sec. IX. Typical cases of the specific examples of gauge transformations that have caused controversy in the literature are worked out in an appendix.

II. FORMULATION OF GENERALIZED HAMILTONIAN DYNAMICS ON $T^*Q \oplus TQ$

The Euler–Lagrange equations for a mechanical system with configuration space Q and described by the Lagrangian L: $TQ \to R$ are completely equivalent,[15] even when the Lagrangian is degenerate, to the canonical equations of motion (4) or (5) on the Whitney sum $W_0 = T^*Q \oplus TQ$, with canonical projection pr_i on the ith factor, of phase space T^*Q and velocity space TQ. In those equations, $X \in TW_0$ is the extended velocity vector with components $(\dot q^i, \dot p_j, \dot v^k)$ relative to the natural bundle chart on TW_0 induced by that with coordinates (q^i, p_j, v^k) on W_0, the canonical 1- and 2-forms are

$$\theta = \mathrm{pr}_1^*\cdot\theta_Q \quad \text{and} \quad \omega = \mathrm{pr}_1^*\cdot\omega_Q \tag{1}$$

with

$$\theta_Q = \pi_Q^*\colon\ T^*Q \to T^*T^*Q \quad \text{and} \quad \omega_Q = -d\theta_Q, \tag{2}$$

and D is the dynamical function

$$D\colon\ W_0 \to R\colon\ w \mapsto \langle \mathrm{pr}_1\cdot w | \mathrm{pr}_2\cdot w\rangle - L\cdot\mathrm{pr}_2\cdot w. \tag{3}$$

The canonical equation of motion is

$$i(X)\cdot\omega = dD \tag{4}$$

and is equivalent to the two equations

$$\mathbf{L}_X\cdot\theta = d\cdot L\cdot\mathrm{pr}_2 \quad \text{and} \quad \pi_{Q*}\cdot\mathrm{pr}_{1*}\cdot X = \mathrm{pr}_2, \tag{5}$$

the latter being the second-order equation condition.

The equation of motion cannot be satisfied at every point of W_0: In the degenerate Lagrangian case, the equation holds only on the final constraint submanifold S upon which the equation of motion possesses consistent solutions, a consistent solution X being a solution that does not describe

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motions leading off S. Thus, a consistent solution X lies in $\underline{TS}$: $= j_{S*} \cdot TS$ with $\underline{S} = j_S \cdot S$ and j_S the inclusion of S in W_0. There exist a number of procedures[1,4,5,16] for calculating the final constraint submanifold.

The equation of motion does not have, in general, a unique consistent solution in the degenerate Lagrangian case: If X is one smooth consistent solution and Y any smooth vector field such that $Y|_{\underline{S}} \in \ker \omega \cap \underline{TS}$, then $X + Y$ is also a smooth consistent solution. The difference between any two consistent solutions is a vector field on $\underline{S}$ with values in, and such differences span,

$$V = \ker \omega \cap \underline{TS}. \tag{6}$$

III. TIME-DEPENDENT FORMALISM

A vector field in V on $\underline{S}$ generates through its flow a map that, for an infinitesimal time, leaves the physical state unchanged. One cannot conclude from this, however, that a finite flow of a vector field Y in V on $\underline{S}$ is a transformation that leaves the physical state unchanged since (with X a consistent solution to the equation of motion) it is $X + Y$ that must be considered, not Y alone. For example, the flow $\Phi_t^{(+)}$ from time 0 to time t generated by $X + Y$ is not necessarily the flow Φ_t generated by X alone followed by the flow Φ_t^Y generated by Y alone.

In order then to discuss the transformations that change X into $X + Y$, we must take the time into account and work with

$$W = T^*Q \oplus TQ \times R \tag{7}$$

with t, the coordinate on R, equal to the curve parameter of X and with canonical projection pr_W: $W \rightarrow W_0$. The solution X is modified to $\widetilde{X} \in TW$ such that $\mathrm{pr}_{W*} \cdot \widetilde{X} = X$ by the addition of a time component with $\langle dt | \widetilde{X} \rangle = 1$. The extra component in $\widetilde{X}$ allows one to take account, by means of $\mathbf{L}_{\widetilde{X}}$, of rates of change due to an explicit time dependence, as well as variations with time due to motions in $T^*Q \oplus TQ$.

Any Y in TW_0 can be lifted uniquely to a vector $\overline{Y}$ in TW by

$$\bar{\ }: TW_0 \rightarrow TW \quad \text{with} \quad \mathrm{pr}_{W*} \cdot \overline{Y} = Y \ \text{and} \ \langle dt | \overline{Y} \rangle = 0. \tag{8}$$

Let the zero vector field in R be designated $\{\vec{0}\}$, so $\overline{Y} \in \overline{TW}_0$ where, for any space M, $\overline{M} = M \times \{\vec{0}\}$. Also, any function f on W_0 can be lifted uniquely via the map

$$\mathrm{pr}_W: \ W_0 \times R \rightarrow W_0: \ (w_0, t) \mapsto w_0 \tag{9}$$

to a function $\bar{f}$ on W by

$$\bar{\ }: \mathscr{F}(W_0) \rightarrow \mathscr{F}(W): \ f \mapsto \bar{f} = f \cdot \mathrm{pr}_W. \tag{10}$$

The equation of motion in the time-dependent formalism is, on W,

$$i(\widetilde{X}) \cdot \omega_D = 0$$

with

$$\omega_D = \widetilde{\omega} + d\overline{D} \wedge dt \ \text{and} \ \widetilde{\omega} = \mathrm{pr}_w^* \cdot \omega. \tag{11}$$

IV. GENERAL PROPERTIES OF THE GENERATORS OF GAUGE TRANSFORMATIONS

Let G be a vector field

$$G: \ W_0|_{\underline{S}} \times R \rightarrow TW_0|_{\underline{S}} \times TR \tag{12}$$

that generates diffeomorphisms that transform a consistent solution $\widetilde{X}$ into $\widetilde{X} + \overline{Y}$ with $\overline{Y}$ a vector field in $\overline{V}$. The transformations must not generate motions off the final constraint submanifold so that G is tangent to $\underline{S} \times R$. The transformations must leave the time parametrization unchanged so $\mathbf{L}_G t = 0$, and therefore $G \in \overline{\underline{TS}}$. The equation of motion must remain unchanged in form so G satisfies, on $\underline{S} \times R$, $\mathbf{L}_G \cdot \widetilde{\omega} = dK \wedge dt$ for some function K on W. Thus, G is the generalization to the Whitney sum $T^*Q \oplus TQ$ of the generator of a canonical transformation on T^*Q.

Our interest here does not lie, however, in general canonical transformations, being restricted to only those that change $\widetilde{X}$ by the addition of a $\overline{Y}$ in $\overline{V}$. Thus, we impose the condition that

$$\mathbf{L}_G \widetilde{X} \in \overline{V} \tag{13}$$

for every solution $\widetilde{X}$ of the canonical equation of motion.

The possible differences $\widetilde{X} - \widetilde{X}'$ between any two consistent solutions $\widetilde{X}$ and $\widetilde{X}'$ span $\overline{V}$ and so, since $\mathbf{L}_G(\widetilde{X} - \widetilde{X}') \in \overline{V}$, we have that

$$\mathbf{L}_G \overline{Y} \in \overline{V} \quad \text{for any vector field } Y \text{ in } V. \tag{14}$$

This condition and (13) for *one* particular solution of the equation of motion are equivalent to (13) for *every* solution $\widetilde{X}$ of the canonical equation. Furthermore, for any G' and G'' satisfying the conditions for G given above, we obtain

$$\mathbf{L}_{[G',G'']} \widetilde{X} = \mathbf{L}_{G'}(\mathbf{L}_{G''} \widetilde{X}) - \mathbf{L}_{G''}(\mathbf{L}_{G'} \widetilde{X}) \in \overline{V}. \tag{15}$$

Hence the set of such G's is closed under commutation.

We call a *gauge generator* any vector field G that is a canonical transformation and satisfies (13) and $\mathscr{G}$ the set of all gauge generators. The flows generated by an element G of $\mathscr{G}$ we call *gauge transformations*. Note that the generators of gauge transformations may be defined only on $\underline{S} \times R$.

That such transformations are generalizations of the usual gauge transformations can be seen from the following: Consider local natural bundle coordinates $\{q^i, p_j, v^l, t\}$. Then, on $\underline{S} \times R$

$$\mathbf{L}_G v^i = \mathbf{L}_G \mathbf{L}_{\widetilde{X}} q^i = \mathbf{L}_{\widetilde{X}} \mathbf{L}_G q^i \tag{16}$$

because of (13). Thus, the gauge transform of v^i is the time derivative of that of q^i. Moreover, G lies in $\overline{\underline{TS}}$ so, in particular, on $\underline{S} \times R$

$$\mathbf{L}_G \cdot \left(p_i - \frac{\partial L}{\partial v^i} \right) = 0; \tag{17}$$

under a gauge transformation, the transform of p_i can be obtained from that of $\partial L / \partial v^i$. Finally, we have from the equation of motion in the form (5) that, on $\underline{S} \times R$,

$$\begin{aligned} &\mathbf{L}_G \cdot (L \cdot \mathrm{pr}_2 \cdot \mathrm{pr}_w) \\ &\quad = \mathbf{L}_{\widetilde{X}} \cdot i(G) \cdot \mathrm{pr}_W^* \cdot pr_2^* \cdot \theta_Q - i([\widetilde{X}, G]) \cdot \mathrm{pr}_W^* \cdot \mathrm{pr}_2^* \cdot \theta_Q \\ &\quad = \frac{d}{dt} \langle \mathrm{pr}_2^* \cdot \theta | \mathrm{pr}_{W*} \cdot G \rangle \end{aligned} \tag{18}$$

so the gauge transform on $\underline{S}$ of the Lagrangian is a perfect time derivative.

V. GAUGE GENERATORS AND FIRST CLASS CONSTRAINTS

We investigate further the condition for gauge transformations that distinguish them from other canonical transformations. That condition, Eq. (13), is equivalent to

$$i([G, \widetilde{X}])\cdot\widetilde{\omega}|_{\underline{S}\times R} = 0 \qquad (19)$$

for every consistent solution $\widetilde{X}$ of the equation of motion, or equivalent to (14) and (19) for one consistent solution $\widetilde{X}$.

The condition (19) can be transformed by using the identity, for vector fields A and B,

$$i([A, B]) = \mathbf{L}_A\cdot i(B) - i(B)\cdot\mathbf{L}_A \qquad (20)$$

on extensions $\widetilde{X}^+$ and G^+ of $\widetilde{X}$ and G to local vector fields on W. {An appropriate extension for $\widetilde{X}^+$ in a natural bundle chart is given by the solution to

$$i(\widetilde{X}^+)\cdot\widetilde{\omega} = [d\overline{D} - (\langle dD\,|\partial/\partial v^i\rangle\cdot \mathrm{pr}_W)dv^i] \qquad (21)$$

that satisfies $\langle dt\,|\widetilde{X}^+\rangle = 1$ and reduces to $\widetilde{X}$ on $\underline{S}\times R$.} Equation (19), independently of the extensions, is equivalent to

$$-i(\widetilde{X})\cdot d\cdot i(G^+)\cdot\widetilde{\omega} + d\,\langle d\overline{D}\,|G^+\rangle = 0 \qquad (22)$$

on $\underline{S}\times R$, since G is tangent to W_K.

This condition can be rewritten: Evaluating (22) on any local vector field $Z\in \underline{TS}$, with extension Z^+, and using the definition of the exterior derivative gives, on $\underline{S}\times R$,

$$-\tfrac{1}{2}\{\widetilde{X}\cdot[\widetilde{\omega}(G^+, Z^+)] - Z\cdot\langle d\overline{D}\,|G^+\rangle - \omega(G, [\widetilde{X}, Z])\} = 0. \qquad (23)$$

The left-hand side of this equation appears on $\underline{S}\times R$ in $d\widetilde{\omega}(\widetilde{X}, G, Z)$ as given by the definition of the exterior derivative of the closed 2-form $\widetilde{\omega}$:

$$\tfrac{1}{3}\{\widetilde{X}\cdot[\widetilde{\omega}(G^+, Z^+)] - G\cdot\langle d\overline{D}\,|Z^+\rangle + Z\cdot\langle d\overline{D}\,|G^+\rangle + \langle d\overline{D}\,|[G, Z]\rangle - \widetilde{\omega}([Z, \widetilde{X}], G)\}|_{\underline{S}\times R} = 0. \qquad (24)$$

Therefore, on $\underline{S}\times R$,

$$\mathbf{L}_G\langle d\overline{D}\,|Z^+\rangle - \langle d\overline{D}\,|\mathbf{L}_G Z\rangle = 2\mathbf{L}_Z\langle d\overline{D}\,|G^+\rangle = \langle \mathbf{L}_G d\overline{D}\,|Z^+\rangle = \mathbf{L}_Z\langle d\overline{D}\,|G^+\rangle = 0, \qquad (25)$$

so $\langle d\overline{D}\,|G^+\rangle$ is a local constraint[17] on $\underline{S}\times R$, equaling a constant there. Moreover, $\langle d\overline{D}\,|G^+\rangle$ is a first class function[17] on $\underline{S}\times R$ since, as shown in the following paragraph, $\overline{Y}\cdot\langle d\overline{D}\,|G^+\rangle|_{\underline{S}\times R} = 0$ for every $Y\in TS^{\perp}$.

We use the definition of $TS^{\perp}$: Let Z be a vector field such that $Z|_{\underline{S}}\in\underline{TS}$ so $i(\overline{Z})\cdot i(\overline{Y})\cdot\widetilde{\omega}|_{\underline{S}\times R} = 0$. Since $G\in\overline{\underline{TS}}$,

$$\begin{aligned}0 &= \mathbf{L}_G\cdot i(\overline{Z})\cdot i(\overline{Y})\cdot\widetilde{\omega}|_{\underline{S}\times R}\\ &= [i(\mathbf{L}_G\overline{Z})\cdot i(\overline{Y})\cdot\widetilde{\omega} + i(\overline{Z})\cdot i(\mathbf{L}_G\overline{Y})\cdot\widetilde{\omega} + i(\overline{Z})\cdot i(\overline{Y})\cdot\mathbf{L}_G\widetilde{\omega}]|_{\underline{S}\times R}.\end{aligned} \qquad (26)$$

The first term is zero as $\mathbf{L}_G\overline{Z}\in\overline{\underline{TS}}$. To evaluate the third term, we use $\mathbf{L}_G\cdot\widetilde{\omega} = dK\wedge dt$ and the equation of motion on $\underline{S}$: Since on $\underline{S}\times R$

$$\begin{aligned}\mathbf{L}_G\cdot i(\widetilde{X})\cdot\widetilde{\omega} &= i(\widetilde{X})\cdot\mathbf{L}_{G^+}\cdot\widetilde{\omega} = \langle dK\,|\widetilde{X}\rangle\,dt - dK\\ &= \mathbf{L}_{G^+}\cdot d\overline{D} = d\,\langle d\overline{D}\,|G^+\rangle,\end{aligned} \qquad (27)$$

$$i(\overline{Z})\cdot i(\overline{Y})\cdot\mathbf{L}_{G^+}\cdot\widetilde{\omega} = -i(\overline{Z})\cdot i(\overline{Y})\cdot d\,\langle d\overline{D}\,|G^+\rangle\wedge dt = 0 \qquad (28)$$

on $\underline{S}\times R$. Therefore, from (26), $\mathrm{pr}_{W*}\cdot\mathbf{L}_{G^+}\overline{Y}|_{\underline{S}\times R}\in\overline{TS}^{\perp}$ and hence

$$\overline{Y}\cdot\langle d\overline{D}\,|G^+\rangle|_{\underline{S}} = G\cdot\langle d\overline{D}\,|\overline{Y}\rangle|_{\underline{S}} + i([\overline{Y}, G])\cdot d\overline{D}\,|_{\underline{S}\times R} = 0, \qquad (29)$$

as $G\in\underline{TS}$ and $\langle d\overline{D}\,|\,\overline{TS}^{\perp}\rangle|_{\underline{S}} = 0$.

Thus, it follows from (13) that $\langle d\overline{D}\,|G^+\rangle$ is a (local) first-class constraint on $\underline{S}$.

VI. GAUGE GENERATORS IN $(TS^{\perp}\cap\underline{TS})\times\{\vec{0}\}$

The set $\mathscr{G}$ of gauge generators G yields first-class constraints $\langle d\overline{D}\,|G^+\rangle$, as does each element Y whose restriction on $\underline{S}$ lies in

$$\mathfrak{G} = TS^{\perp}\cap\underline{TS}\times\{\vec{0}\} \qquad (30)$$

[where $TS^{\perp}$ is the set of all vectors Z such that $j_S^*\cdot i(Z)\cdot\omega = 0$], since Y generates a first-class constraint ϕ through[18] $i(Y)\cdot\widetilde{\omega} = d\phi$. However, $\mathscr{G}$ may contain elements not in $\mathfrak{G}$, as the example $G = \partial/\partial q$ for the one-dimensional system on $Q = R$ with $L = \frac{1}{2}v^2 + q$ demonstrates. Nevertheless, $\mathfrak{G}$ and $\{\widetilde{X}, Y\in\mathfrak{G}\}$ are closed, as the following arguments show, so we might expect that there is a subalgebra of $\mathscr{G}$ that lies in $\mathfrak{G}$. We determine this subalgebra in this section.

To show that $\mathfrak{G}$ is closed, let X and Y be vector fields that on restriction to $\underline{S}\times R$ lie in $\mathfrak{G}$ and Z be a vector field with $Z|_{\underline{S}\times R}\in\overline{\underline{TS}}$. The fact that $\widetilde{\omega}$ is closed gives, on $\underline{S}\times R$, $\widetilde{\omega}([X, Y], Z) = 0$ since $\underline{TS}$ is closed under commutation. Therefore, $\mathfrak{G}$ is closed under commutation. With $\widetilde{X}^+$ any extension of a consistent solution of the equation of motion, the definition of $d\widetilde{\omega}(X^+, Y, Z)$, which is zero, gives on $\underline{S}\times R$

$$\begin{aligned}0 &= -Y\cdot\langle d\overline{D}\,|Z\rangle - \widetilde{\omega}([\widetilde{X}, Y], Z) + \langle d\overline{D}\,|[Y, Z]\rangle\\ &= -Z\cdot\langle d\overline{D}\,|Y\rangle - \widetilde{\omega}([\widetilde{X}, Y], Z)\\ &= -\widetilde{\omega}([\widetilde{X}, Y], Z)\end{aligned} \qquad (31)$$

so that $\{\widetilde{X}, Y\in\mathfrak{G}\}$ is closed under commutation.

To calculate the elements in $\mathfrak{G}$, we expand the extension G^+ of an element G of $\mathfrak{G}$ in a set, to be selected shortly, of basis vectors $\{Z^A\}_{A=1,2,\ldots,3N}$ for $\underline{TW}_0$:

$$G^+ = b_A Z^A \quad \text{with } b_A\colon W\to R. \qquad (32)$$

Equating (22), with this expansion, to zero gives, on $\underline{S}\times R$, with $\mathbf{L}_{\widetilde{X}}\cdot b_A = \dot{b}_A$,

$$\dot{b}_A i(Z^A)\cdot\widetilde{\omega} = b_A d\,\langle d\overline{D}\,|Z^A\rangle - b_A i(\widetilde{X})\cdot d\cdot i(Z^A)\cdot\widetilde{\omega}. \qquad (33)$$

In the following, we show how to solve this equation for those G that involve local vector fields in $\mathfrak{G}$, which contains $\overline{V}$ (cf. the first paragraph of Sec. III). The method of solution relies heavily on the local calculation of the final constraint manifold described in Sec. IIIB of Ref. 1.

A. Choice of basis vectors for $\mathfrak{G}$

Take, then, for the first dim V of the Z^A's, a set of local vector fields $\{\overline{Y}^{\alpha 1}\}$, where the set $\{Y^{\alpha 1}\}|_{\underline{S}\times R}$ spans V locally on $\underline{S}$. Then, on $\underline{S}\times R$,

$$i(\overline{Y}^{\alpha 1})\cdot\widetilde{\omega} = 0 \quad\text{and}\quad \langle d\overline{D}\,|\overline{Y}^{\alpha 1}\rangle = \langle dD\,|Y^{\alpha 1}\rangle\cdot\mathrm{pr}_W. \qquad (34)$$

But the $Y^{\alpha 1}$'s generate sets $\{Y^{\alpha 2}\}$ and so on through relations involving $i(Y)\cdot\omega$'s and $\langle dD\,|Y\rangle$'s, as described in Sec. IIIB of Ref. 1.

The form of Eq. (33) suggests that we consider the equation

$$i(Y^{\overline{\alpha}})\cdot\omega = d\,\langle dD\,|Y^{\alpha}\rangle \qquad (35)$$

and ask if, for $Y^{\alpha}|_{\underline{S}}$ in $TS^{\perp}\cap TS$, there exists a solution $Y^{\overline{\alpha}}$ such that $Y^{\overline{\alpha}}|_{\underline{S}}$ lies in $\underline{TS}$. (Such a solution would also lie in

$TS^{\perp}$ because of the equation that it satisfies.) By a theorem due to Gotay, Nester, and Hinds,[5] there does exist such a solution if, on $\underline{S}$, $\langle d\langle dD|Y^{\alpha}\rangle|TS^{\perp}\rangle = 0$. We now show that this relation is satisfied for the Y^{α} of interest here.

Let Y be any local vector field in $TS^{\perp}$. Then, on $\underline{S}$,

$$\begin{aligned} i(Y)\cdot d\cdot i(Y^{\alpha})\cdot dD &= i(Y^{\alpha})\cdot \mathbf{L}_Y\cdot dD + i([Y, Y^{\alpha}])\cdot dD \\ &= i([Y, Y^{\alpha}])\cdot dD. \end{aligned} \tag{36}$$

This last term is a constraint function vanishing on $\underline{S}$ if $[Y, Y^{\alpha}]$ on $\underline{S}$ lies in $TS^{\perp}$. To show that the latter is true, let Z be any local vector field such that $Z|_{\underline{S}} = j_{K*}\cdot Z_K$. Then, on $\underline{S}$,

$$\begin{aligned} i(Z)\cdot i([Y, Y^{\alpha}])\cdot\omega = &- \mathbf{L}_{Y^{\alpha}}\cdot[i(j_{K*}\cdot Z_K)\cdot i(Y)\cdot\omega] \\ &+ i(\mathbf{L}_{Y^{\alpha}}j_{K*}\cdot Z_K)\cdot i(Y)\cdot\omega \\ &+ i(j_{K*}\cdot Z_K)\cdot i(Y)\cdot \mathbf{L}_{Y^{\alpha}}\cdot\omega \\ = &\, i(j_{K*}\cdot Z_K)\cdot i(Y)\cdot d\cdot i(Y^{\alpha})\cdot\omega \end{aligned} \tag{37}$$

since Y^{α} lies in $\underline{TS}$ and Y in $TS^{\perp}$. The last expression in (37) vanishes if, on $\underline{S}$, $i(Y^{\alpha})\cdot\omega = d\phi$ for some ϕ. Since Y^{α} in $\ker\omega\cap\underline{TS}$ does satisfy[18] an equation of this form, there exists a solution $Y^{\bar{\alpha}}$ to (35) that is tangent to S.

Thus, we can start with a minimal set of local vector fields $\{Y^{\bar{a}1}\}$ (suitably selected, as described below) that span $\ker\omega\cap\underline{TS}$ and generate by

$$i(Y^{\bar{a}j})\cdot\omega = d\langle dD|Y^{\bar{a}j-1}\rangle, \tag{38}$$

with $Y^{\bar{a}j}$ in $\underline{TS}$, a sequence of vector fields $\{Y^{\bar{a}1}\}$ that, on $\underline{S}$, lie in $\ker\omega\cap\underline{TS}$. The vector fields resulting from this procedure are the only ones generated by $\{Y \text{ in } \ker\omega\cap\underline{TS}\}$ and therefore (see the first paragraph of Sec. III) appear at first glance to be the only ones needed in discussions of gauge invariance and of Dirac's conjecture (see Sec. VII). This is misleading, though, since the zero vector lies in V so the condition $\mathbf{L}_G\tilde{X} = 0$ may apply to certain gauge generators. These arise from those $Y^{\bar{a}j-1}$ for which $d\langle dD|Y^{\bar{a}j-1}\rangle$ is zero on $\underline{S}$.

Notice that if the differential of $\langle dD|Y^{\bar{a}j-1}\rangle$, or a linear combination of these, vanishes, then the corresponding $Y^{\bar{a}j}$ that lies in $\underline{TS}$ is zero. In this case, one linearizes those particular constraint functions and looks for a linear combination, say ϕ^j, with a finite nonzero differential on $\underline{S}$ and such that a solution Y^j of

$$i(Y^j)\cdot\omega = d\phi^j \tag{39}$$

exists that is tangent to S. Then one calculates Y^{j+1} from an equation similar to (35) and continues on. The procedure is similar to that described below; an example is given in the Appendix. In any event, we take the $\overline{Y}^{aj}$'s and $\overline{Y}^{j}$'s as a basis[18] for $\mathfrak{G}$.

Note that dim $\ker\omega\cap\underline{TS}$ need not equal dim-$\ker\omega\cap TW_1$: On the one hand, a vector field in $\underline{TW_1}|_{\underline{S}}$ need not lie in $\underline{TS}$ whereas, on the other, a vector field can lie in $\underline{TS}$, and so in $\underline{TW_1}|_{\underline{S}}$, but not in $\underline{TW_1}|_{W_1}$.

B. Calculation of gauge generators in $\mathfrak{G}$

Let us assume that there is no $Y^{\bar{a}j}$ such that $\langle dD|Y^{\bar{a}j}\rangle$ yields an independent constraint and $d\langle dD|Y^{\bar{a}j}\rangle = 0$. (This assumption is made only to keep the equations in manageable form; it is straightforward in a specific case where this assumption does not hold to generalize the method given below.) Then, we set the Z^A for a limited range of A equal to a suitable set of basis vectors for $\ker\omega\cap\underline{TS}$, selected in the following manner. Let $\{Y^{aK+1}\}_{a=1,\ldots,m_{K+1}}$ be a linearly independent set of vectors that span $\{Y^{\bar{a}K+1}\}$. Then we can write on $\underline{S}$

$$i(Y^{aK+1})\cdot\omega = d\langle dD|Y^{a'K}\rangle \tag{40}$$

for some linearly independent $Y^{a'K}$ in the span of $\{Y^{\bar{a}K}\}$. Let m_K be the dimension of the span of $\{Y^{\bar{a}K}\}$. The $(m_K - m_{K+1})$ vectors $\{Y^{a''K}\}$ needed to form, with $\{Y^{a'K}\}$, a basis $\{Y^{aK}\}$ for the span of $\{Y^{\bar{a}K}\}$ may be chosen so that each $\langle dD|Y^{a''K}\rangle$ is a linear combination of the $\langle dD|Y^{a'K}\rangle$ and $\langle dD|Y^{\bar{a}j}\rangle$ for $j<K$. Repeat the process with $\{Y^{aK}\}$ replacing $\{Y^{aK+1}\}$, and so on. Thus, we obtain a set $\{Y^{aj}\}$ that forms a basis for the span of $\{Y^{\bar{a}j}\}$ with

$$i(Y^{aj+1})\cdot\omega = d\langle dD|Y^{aj}\rangle,$$
$$a = 1,\ldots,m_{j+1} \quad\text{and}\quad j = 1,2,\ldots,K, \tag{41}$$

and

$$\langle dD|Y^{aj}\rangle = C^{aj}_{bi}\langle dD|Y^{bi}\rangle,\quad j = 1,2,\ldots,K+1,$$
$$a = m_{j+1}+1,\ldots,m_j,\quad i = 1,2,\ldots j\quad b = 1,2,\ldots,m_{i+1}. \tag{42}$$

Note that $m_{K+2} = 0$.

We now expand G on $\underline{S}\times R$ as

$$G = \sum_{j=1}^{K+1}\sum_{a=1}^{m_j} b_{aj}\overline{Y}^{aj} \tag{43}$$

with the b_{aj} functions on $\underline{S}\times R$ that are to be determined as far as possible by Eq. (33):

$$\begin{aligned} &\sum_{j=1}^{K+1}\sum_{a=1}^{m_j}\dot{b}_{aj}i(\overline{Y}^{aj})\cdot\omega \\ &= \sum_{j=1}^{K}\sum_{a=1}^{m_{j+1}}\dot{b}_{aj+1}d\langle dD|Y^{aj}\rangle\cdot \mathrm{pr}_W \\ &= \sum_{j=1}^{K}\sum_{a=1}^{m_{j+1}} b_{aj}d\langle dD|Y^{aj}\rangle\cdot\mathrm{pr}_W \\ &\quad+\sum_{j=1}^{K+1}\sum_{a=m_{j+1}+1}^{m_j} b_{aj}\sum_{i=1}^{j}\sum_{b=1}^{m_{i+1}} C^{aj}_{bi}d\langle dD|Y^{bi}\rangle\cdot\mathrm{pr}_W \\ &= \sum_{j=1}^{K}\sum_{a=1}^{m_{j+1}}\left(b_{aj} + \sum_{i=j}^{K+1}\sum_{b=m_{i+1}+1}^{m_i} b_{bi}C^{bi}_{aj}\right) \\ &\quad\times d\langle dD|Y^{aj}\rangle\cdot\mathrm{pr}_W. \end{aligned} \tag{44}$$

Thus, for $j\leqslant K$ and $1\leqslant a\leqslant m_{j+1}$,

$$\dot{b}_{aj+1} = b_{aj} + \sum_{i=j}^{K+1}\sum_{b=m_{i+1}+1}^{m_i} b_{bi}C^{bi}_{aj}. \tag{45}$$

The b_A's are also subject to the condition (14) so, for any vector field Y in V,

$$\sum_{j=1}^{K+1}\sum_{a=1}^{m_j}\{(\overline{Y}\cdot b_{aj})\overline{Y}^{aj} + b_{aj}[\overline{Y},\overline{Y}^{aj}]\}\in\overline{V}. \tag{46}$$

However, since

$$\begin{aligned} i([Y^{aj}, Y^{bi}])\cdot\omega &= \mathbf{L}_{Y^{aj}}\cdot i(Y^{bi})\cdot\omega - i(Y^{bi})\cdot\mathbf{L}_{Y^{aj}}\cdot\omega \\ &= d\cdot i(Y^{aj})\cdot d\langle dD|Y^{bi-1}\rangle, \end{aligned} \tag{47}$$

$[Y, Y^{aj}] \in V$ so that the b_A's are restricted by

$$\overline{Y} \cdot b_{aj} = 0 \quad \text{for every} \quad Y \in V. \tag{48}$$

The $m_{K+1} b_{a\,K+1}$ are arbitrary save for the above condition, as are the $(m_j - m_{j+1}) b_{aj}$ with $a > m_{j+1}$ and $j \leqslant K$. Thus, there are a total of

$$m_{K+1} + (m_K - m_{K+1}) + \cdots + (m_1 - m_2) = m_1 \tag{49}$$

independent and essentially arbitrary b_{aj}'s; the rest of them are determined by (45) to have the form

$$b_{aj} = b_{aj}(\ldots, \ddot{b}_{bi}, \dot{b}_{bi}, b_{bi}), \quad a \leqslant m_{j+1} \text{ and } b > m_{i+1}. \tag{50}$$

If some $\langle dD \,|\, Y^{aj} \rangle$ were zero, the equation corresponding to Eq. (45) would give $\dot{b}_{a\,j+1} = 0$, in which case one is dealing with what corresponds in gauge field theory to a global, as compared to a local, gauge invariance. Here, we call a *local* gauge generator one that involves arbitrary functions of the time and a *global* gauge generator one that does not. Examples of both are given in the Appendix.

VII. DIRAC'S CONJECTURE[14]

The discussions that have appeared in the literature of the gauge transformations of generalized dynamics have been based on a time-independent formalism similar to that in Ref. 1. We can compare the basis for those discussions with the present work by evaluating at one instant of time, say $t = t_0$, some of the results derived above.

At any one given instant of time, the values of a smooth but otherwise arbitrary time-dependent function and its time derivatives are independent of each other. Thus, Eq. (33) does not yield any condition restricting the values of the expansion coefficients b_A of basis vectors Z^A of $\mathfrak{G}|_{t_0}$ for an element $G|_{t_0}$ of $\mathscr{G}|_{t_0}$:

$$G|_{t_0} = b_A Z^A, \quad b_A \colon \underline{S} \times \{t_0\} \to R, \tag{51}$$

where each b_A satisfies the restriction (48) but is otherwise arbitrary. Also, there is no distinction at one instant of time between global and local gauge transformations [see the discussion below Eq. (50)] since they are distinguished solely by their time dependence.

Considerations of infinitesimal gauge transformations within the time-independent formalism led Dirac to conjecture that the generalization of the Hamiltonian on T^*Q should be modified through the addition of arbitrary combinations of all of the first-class constraints, corresponding here to the addition of $b_{aj} \langle dD \,|\, Y^{aj} \rangle$ (or possibly $b_{aj} \langle dD \,|\, Y^{aj} \rangle + b_j \phi_j$) to D, with each b_{aj} (and b_j) arbitrary. Certainly, the dynamical function (the generalization on $T^*Q \oplus TQ$ of the Hamiltonian) is modified by an infinitesimal gauge transformation at time t_0 through the addition of an arbitrary infinitesimal linear combination of the first-class constraints as determined by the action of a vector $G|_{t_0}$ of $\mathfrak{G}|_{t_0}$ on $\overline{D}$:

$$\mathbf{L}_G \overline{D}|_{t_0} = b_A \langle d\overline{D} \,|Z^A \rangle. \tag{52}$$

Note, however, that the exterior derivative, which appears in the equation of motion, of some of the terms in the expansion may vanish on $\underline{S} \times \{t_0\}$, so not all first-class constraints contribute to a modification of the equation of motion.

Dirac's conjecture is equivalent to requiring that the solutions of the equation of motion can be determined only up to elements in $\mathfrak{G}$ (and not just its subspace $\overline{V}$, as follows from the arguments given in the present study). And, in fact, at one instant t_0 of time, a consistent solution X may be modified by an almost arbitrary linear combination of the basis vectors in $\mathfrak{G}$ since X is transformed under the gauge generator $G = \overline{g}$ with $g \in \underline{TS}$ to $X + \epsilon \mathbf{L}_g X$, where ϵ is small, and

$$\mathbf{L}_g X - \dot{b}_A Z^A \in \overline{V} \tag{53}$$

by Eq. (13). The arbitrariness is limited by the fact that the expansion in (53) does not contain any generator Z^A of a global gauge transformation whose coefficient b_A has zero time derivative or, equivalently, that is determined by a first class constraint $\langle dD \,|\, Y \rangle$ such that $d \langle dD \,|\, Y \rangle = 0$.

Thus, Dirac's conjecture is correct in that, at one instant of time, the dynamical function is determined only up to an arbitrary linear (infinitesimal) combination of the first-class constraints in the form $\langle dD | Z^A \rangle$ or, equivalently, a consistent solution $\widetilde{X}$ is determined only to within an (almost) arbitrary linear combination, with small coefficients for elements of $\mathfrak{G}/\overline{V}$, of basis vectors in $\mathfrak{G}$. However, to achieve these modifications does not require one to alter the equation of motion one bit: The result is contained within the time-dependent formalism given above or that which would be obtained from the time-independent formulation on T^*Q given in Ref. 1. That is, one need not add arbitrary time-dependent linear combinations of the first-class constraints to the dynamical function (or of the first class secondary constraints to the generalized Hamiltonian on T^*Q): The proper combinations are already there.

Adding such linear combinations enlarges the group of gauge transformations from elements of the form $b_A Z^A$ with the b_A's related by equations like (45) to elements of that form with no restrictions on the b_A's. In general, this is different than transforming a global gauge generator, for which the b_A's satisfy an equation like (45), to the corresponding local gauge generator.

Dirac's conjecture has resulted in numerous discussions, based on a time-independent formalism, in the literature.[5-13] Some of these are based on particular Lagrangians and concern those gauge transformations that are called global here.

Global gauge transformations can be considered to correspond to that part of a local gauge invariance that is left over after the imposition of a gauge condition. This explains why Gotay and Nester,[5,6,10,12] although their time-independent study did not involve the distinction given here between local and global gauge transformations, raised the question, stated here in the language of the present work, of the physical interpretation of the mechanics—does one interpret a system with a global gauge invariance as representing a system with a local gauge invariance upon which a gauge condition has been applied, or not? This question is beyond the scope of the present work, which is concerned only with determining the gauge transformations, local or global, for a given Lagrangian, and thus a unique physical interpretation for the system described by that Lagrangian.

Some of this discussions in the literature have centered around specific Lagrangians. The gauge transformations for two typical cases are calculated within the present formalism, and discussed, in the Appendix. (The other class of such specific Lagrangians is discussed in the Appendix of Ref. 1).

VIII. GAUGE TRANSFORMATIONS ON T^*Q AND TQ

The relationships between the formulations of generalized dynamics on $T^*Q \oplus TQ$, T^*Q, and TQ are described in the preceding paper.[1] That description and the notation used there, with some modifications similar to that used in this paper, provide the basis for the following.

A consistent solution X_1 of the canonical equation of motion on T^*Q is determined only up to elements in $TM_1^{\perp} \cap \underline{TM}_K$. Thus, in the time-dependent formulation on $\overline{T^*Q} \times R$, gauge transformations are defined by the conditions on their generators $\mathscr{G}_1 = \{G_1\}$ that each G_1 lie in $\underline{\overline{TS}}_K$, be a canonical transformation, and satisfy

$$\mathbf{L}_{G_1}\tilde{X}_1 \in \overline{TM}_1^{\perp} \cap \underline{\overline{TM}}_K. \tag{54}$$

The projection $G' = (\mathrm{pr}_{1*} \times id_{R*})\cdot G$ of $G \in \mathscr{G}$ satisfies this equation for G_1: The variation of G along the fibers of $r_K \times id$: $\underline{W}_K \times R \to \underline{M}_K \times R$ is given by Eq. (14). Moreover, $[Y, X] \in \overline{TW}_1^{\perp}$ for $Y \in \overline{V}$. As $\mathrm{pr}_{1*} \times id_{R*}$ extinguishes in G only its terms in $\overline{V}_2$, $\mathbf{L}_{G'}\cdot X_1 \in \overline{TM}_1^{\perp}$.

Moreover, we may go the other way: Given a G_1 satisfying the above conditions, and a cross section σ of the bundle r_K: $\underline{W}_K \to \underline{M}_K$, calculate $(\sigma_* \times id_{R*})\cdot G_1$ and carry it off $(\sigma \times \overline{id})\cdot \underline{M}_K \times R$ to $\underline{W}_K \times R$ by using $\mathbf{L}_G\cdot(X - X\cdot\sigma\cdot\mathrm{pr}_1) \in \overline{V}$. Thus, $\mathrm{pr}_{1*}\cdot\mathscr{G}$ gives $\mathscr{G}_1$.

The relation between the gauge transformations on TQ and those on $T^*Q \oplus TQ$ is even easier to obtain. Because $\overline{\mathbf{FL}}$ is a diffeomorphism, the gauge transformations on $\underline{W}_K \times R$ carry over directly, via pr_2, to $\underline{N}_K \times R$, with gauge generators

$$G_2 = (\mathrm{pr}_{2*} \times id_{R*})\cdot G \tag{55}$$

on $\underline{N}_K \times R$. Notice that the generalized gauge transformations are restricted to the final constraint submanifold $\underline{N}_K \times R$.

IX. SUMMARY AND CONCLUSIONS

Since consistent solutions to the equation of motion are determined only modulo elements in V, any transformation that changes a consistent solution X to $X + Y$, in which the vector field $Y \in V$, is physically unobservable, like a gauge transformation in gauge field theory. Nevertheless, the vector field Y alone does not generate a gauge transformation: The motion starting at a point $w(t_0)$ generated by X and that generated by $(X + Y)$ diverge as time proceeds so, at a later time t, the point $w(t)$ on the flow line of X is not, in general, on that flow line of $X + Y$ that began at $w(t_0)$, even though $X|_{w(t)}$ and $(X + Y)|_{w(t)}$ are defined as vectors in $T_{w(t)}W_0$. Thus, to study the gauge transformations, it is necessary to take layers of copies of TW_0 in time, thereby distinguishing the point w in W_0 at time t_0 from the same point w in W_0 at time $t \neq t_0$. Therefore, it is necessary to work with a time-dependent formulation of generalized dynamics; and this allows an obvious definition of gauge transformations.

A generator G of a gauge transformation in generalized dynamics is a vector field in $\underline{\overline{TS}}$ that generates a canonical transformation and satisfies $\mathbf{L}_G\tilde{X} \in \overline{V}$. This definition is more general than allowed by the discussions of gauge transformations in the literature[5,6,10,12,14] (which for instance do not include the example in Sec. VI) since those discussions deal only with the set of gauge generators that are connected to V.

The value of the time-dependent formulation can be seen by comparing Eqs. (13) and (53): The former leads to explicit expressions for gauge generators, for example, in terms of m_1 arbitrary functions in Sec. VIB, whereas the latter provides little information on g since the value of $\dot{b}_A$ at one instant of time is arbitrary. Furthermore, a time-dependent formulation is necessary to distinguish global from local gauge transformations since, in generalized dynamics, it is their time dependence that separates the two classes.

The discussions in the literature of gauge transformations have been based on time-independent formulations of generalized dynamics, and thus they do not involve that distinction, an omission that has led to some ambiguity. This can be seen by comparing the worked-out examples in the Appendix with the discussions in the original references.

The time-dependent formulation provides a precise form, Eq. (52), for the basis of Dirac's conjecture, but it also shows that the conjecture itself is not needed: The dynamical function (or the generalized Hamiltonian on T^*Q) takes care, with the proper time dependence, of those constraints that are added to D according to (52). And carrying out the conjecture not only changes global to local gauge transformations; it would also decouple those gauge transformations with coupled time dependences [see Eq. (45)].

APPENDIX

The gauge transformations for two typical cases that have been described as problem cases in the literature are calculated below. After the reference and the preliminary calculation given as in the Appendix of Ref. 1, the conditions on the gauge generator and the general form of the gauge generator (with the c_i's being time-independent) are presented. The calculation is followed by a brief discussion (in which H_{gen} denotes the Dirac generalized Hamiltonian on T^*Q).

1. Cawley[7]

$$L = v_x v_z + \tfrac{1}{2}yz^2,$$

$$W_0 = \{x, y, z, p_x, p_y, p_z, v_x, v_y, v_z\},$$

$$TW_0^{\perp}: \frac{\partial}{\partial v_x}, \quad \frac{\partial}{\partial v_y}, \quad \frac{\partial}{\partial v_z},$$

$$W_1: p_x - v_z = 0, \quad p_y = 0, \; p_z - v_x = 0, \quad TW_1^{\perp}: \frac{\partial}{\partial y},$$

$$W_2: z = 0, \quad TW_2^{\perp}: \frac{\partial}{\partial p_z},$$

$$W_3: v_z = 0, \quad \text{so } p_x = 0, \quad TW_3^{\perp}: \frac{\partial}{\partial x},$$

$$T = \alpha\left(\frac{\partial}{\partial p_z} + \frac{\partial}{\partial v_x}\right) + \beta\frac{\partial}{\partial x} + \gamma\frac{\partial}{\partial v_y} + \delta\frac{\partial}{\partial y},$$

$$\tilde{X} = A\frac{\partial}{\partial v_y} + v_x\frac{\partial}{\partial x} + v_y\frac{\partial}{\partial y} + v_z\frac{\partial}{\partial z} + \frac{\partial}{\partial t},$$

α, β, and δ independent of v_y, $\dot{\alpha} = 0$, $\dot{\beta} = \alpha$, $\dot{\delta} = \gamma$,

$$G = c_1\left(\frac{\partial}{\partial p_z} + \frac{\partial}{\partial v_x}\right) + (c_1 t + c_2)\frac{\partial}{\partial x} + \dot{\delta}\frac{\partial}{\partial v_y} + \delta\frac{\partial}{\partial y}.$$

The constraint $\langle dD\,|\partial/\partial y\rangle$ is $\frac{1}{2}z^2$ and the resulting constraint in the form z is seen to lead in W_3 to a global gauge generator involving the time-independent c_1 and c_2. In this case, the Dirac conjecture as clarified in Sec. VII would lead at most to the addition of $c_1 p_x$ to the generalized Hamiltonian on T^*Q ($H_{\text{gen}} = p_z p_x + u p_y$, where p_z is an arbitrary constant and u is an arbitrary function of the time, *not* p_x multiplied by an arbitrary function of the time.

2. Gotay,[10] due to Nester

$$L = [1/(2x)]v_y^2,$$

$$W_0 = \{x, y, p_x, p_y, v_x, v_y\}, \quad TW_0^\perp: \frac{\partial}{\partial v_x}, \frac{\partial}{\partial v_y}$$

$$W_1: p_x = 0, \quad p_y - v_y/x = 0, \quad TW_1^\perp: \frac{\partial}{\partial x},$$

$$W_2: v_y = 0, \quad \text{so } p_y = 0, \quad TW_2^\perp: \frac{\partial}{\partial y},$$

$$T = \alpha\frac{\partial}{\partial v_x} + \beta\frac{\partial}{\partial x} + \gamma\frac{\partial}{\partial y},$$

$$\tilde{X} = A\frac{\partial}{\partial v_x} + v_x\frac{\partial}{\partial x} + \frac{\partial}{\partial t},$$

$$\frac{\partial\beta}{\partial v_x} = 0 = \frac{\partial\gamma}{\partial v_x}, \quad \alpha = \dot{\beta}, \quad \dot{\gamma} = 0,$$

$$G = \dot{\beta}\frac{\partial}{\partial v_x} + \beta\frac{\partial}{\partial x} + c_1\frac{\partial}{\partial y}.$$

Thus $\partial/\partial y$, or the constraint p_y, generates a global gauge transformation, corresponding in the Dirac conjecture to adding $(dc_1/dt)p_y = 0$ to the generalized Hamiltonian on T^*Q, $H_{\text{gen}} = up_x$ with u arbitrary.

This example is similar to one due to Allcock,[11] in which $L = xv_y^2$.

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Transient fields in dispersive media

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The problem addressed in this paper is the determination of transmitted and scattered fields produced by a transient electromagnetic field incident on a three-dimensional body when the body and the surrounding medium are allowed to be dispersive. Instead of decomposing the pulse into its Fourier components, the solution is carried out in the time domain to take advantage of marching-in-time procedures. Maxwell's equations are suitably modified, and the reduction of the problem to the solution of an integral equation for a single tangential vector field is adapted to dispersive media. A simple conductor and a collisionless plasma are studied as examples.

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I. INTRODUCTION

The properties of a medium that determine the propagation of an electromagnetic wave, mainly the permittivity and the conductivity, are a consequence of the average response of the atoms in the medium to the local electromagnetic field. Causality and inertia do not allow this response to be instantaneous, so that the behavior of the medium depends on the frequency of an imposed monochromatic field.

A transient field or pulse can always be decomposed into its Fourier components and in principle we can limit ourselves to the study of monochromatic fields. For broadband pulses this approach may not be practical, and in any case the physical behavior of the pulse is more transparent in the time domain. Also the marching-in-time procedures for numerical solutions of integral equations, which are a consequence of the principle of causality, may show advantages over the solution of large systems of linear algebraic equations that arise in the computations for monochromatic fields. Thus, we want to extend the solutions of scattering problems in the time domain to dispersive media.

In particular, we have shown[1] how the fields scattered by and transmitted into a dielectric can be obtained from a single tangential field defined on the surface of the scatterer. This field obeys a (weakly) singular integral equation of the first kind. This theory applies to transient fields for media of constant permittivity ϵ and permeability μ, and to monochromatic fields in media that can be dispersive and that can have a finite conductivity σ.

In this paper we examine what changes have to be introduced in the time-domain formulation to find the scattered and transmitted fields produced by an electromagnetic pulse incident from a region V_1 onto a conducting body occupying a region V_2 bounded by a surface S. We allow the properties of the two media to be functions of frequency, but not of space within each medium, and we assume that they are constant in time. To avoid unnecessarily complicated equations, we assume that the magnetic permeability differs by a negligible amount from that of free space, μ_0, an assumption that holds in most instances.

In Sec. II we introduce the modifications of Maxwell's equations that allow for dispersion, and we express the electromagnetic fields in terms of their initial values and the jumps on the boundary by means of Green's function for the related scalar wave equation. In Sec. III we discuss the elementary solution of the scalar equation and give two examples, a simple conducting medium and a collisionless plasma. We sketch the derivation of the integral equation for the conductor in Sec. IV, and we examine the plasma problem in Sec. V. We leave for an Appendix the proof that the elementary solution for the simple conductor satisfies the correct equation, and the derivation of some convolution products.

We use the notation developed in Ref. 1, and we borrow from that paper those derivations that apply essentially unchanged to this problem. We stay with the theory of distributions to provide a good mathematical foundation to this discussion.

II. TRANSIENT FIELDS IN DISPERSIVE MEDIA

The form of Maxwell's equations that is valid for distributions and includes initial and boundary conditions is

$$\nabla\cdot\mathbf{D} = \rho + \Delta\,(\hat{n}\cdot\mathbf{D})\delta(S), \tag{1}$$

$$\nabla\cdot\mathbf{B} = \Delta\,(\hat{n}\cdot\mathbf{B})\delta(S), \tag{2}$$

$$\nabla\times\mathbf{E} + \dot{\mathbf{B}} = \Delta\,(\hat{n}\times\mathbf{E})\delta(S) + \mathbf{B}_0\delta(t), \tag{3}$$

$$\nabla\times\mathbf{H} - \dot{\mathbf{D}} = \mathbf{j} + \Delta\,(\hat{n}\times\mathbf{H})\delta(S) - \mathbf{D}_0\delta(t), \tag{4}$$

where $\mathbf{B}_0$ and $\mathbf{D}_0$ are the values at the time $t = 0$ of the corresponding fields, the coefficients of the singular distribution $\delta(S)$ are the jumps of the tangential or normal components of the fields across S, and the sources ρ and $\mathbf{j}$ may include singular terms. The equations for monochromatic fields can be obtained by replacing the time derivatives with multiplication by $-i\omega$ and eliminating the initial-value terms. We assume that the constitutive relation between $\mathbf{B}$ and $\mathbf{H}$ remains unchanged from the one in free space,

$$\mathbf{B} = \mu_0\mathbf{H}. \tag{5}$$

When the permittivity is a function of the frequency of a monochromatic field, we can write,[2] for a linear, uniform, isotropic medium,

$$\mathbf{D}_\omega = \epsilon_\omega\mathbf{E}_\omega. \tag{6}$$

The permittivity has the form

$$\epsilon_\omega = \epsilon_0(1 + \chi_\omega), \tag{7}$$

where ϵ_0 is the free-space permittivity and χ_ω is the susceptibility, which tends to zero as ω tends to infinity.

If we express transient fields in terms of their Fourier components,[3] Eq. (6) leads to

$$\mathbf{D}(\mathbf{x},t) = \epsilon_0\left[\mathbf{E}(\mathbf{x},t) + \int_0^\infty \chi(t')\mathbf{E}(\mathbf{x},t-t')dt'\right], \tag{8}$$

where $\chi(t)$ is the Fourier transform of χ_ω divided by $\sqrt{2\pi}$, that is,

$$\chi(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \chi_\omega \exp(-i\omega t). \tag{9}$$

The electric field is a free field, while the displacement vector includes the effects of the medium; causality restricts the integral in Eq. (8) to start at $t'=0$ and the value of $\mathbf{D}$ at time t does not depend on values of $\mathbf{E}$ at later times. The decomposition of ϵ_ω in Eq. (7) allows for the definition of $\chi(t)$ in Eq. (9) in the sense of functions. For distributions, we can rewrite Eq. (8) in the form

$$\mathbf{D} = \epsilon * \mathbf{E}, \tag{10}$$

where the distribution ϵ can be (informally) represented by

$$\epsilon = \epsilon_0[\delta(t) + \chi(t)]\delta^{(3)}(\mathbf{x}); \tag{11}$$

causality then implies that ϵ vanishes for $t<0$.

When the electromagnetic field for positive t is given in terms of the initial values at $t=0$, it is mathematically convenient to assume that the field vanishes for negative t and has a jump equal to the initial value at $t=0$. This does not imply that the physical field vanishes for negative t, and we cannot determine $\mathbf{D}_0$ from $\mathbf{E}_0$, since $\mathbf{D}_0$ depends on earlier values of $\mathbf{E}$ as seen from Eq. (8).

We assume now that there are no free charges in the medium, and that the current density is given by a generalization of Ohm's law to a dispersive medium,

$$\mathbf{j} = \sigma * \mathbf{E}. \tag{12}$$

We substitute Eqs. (5), (10), and (12) into Eq. (4), which becomes

$$\nabla\times\mathbf{B} - \gamma * \mathbf{E} = \Delta(\hat{n}\times\mathbf{B})\delta(S) - \mu_0\mathbf{D}_0\delta(t), \tag{13}$$

where

$$\gamma = \mu_0(\dot{\epsilon} + \sigma). \tag{14}$$

We now solve these equations by means of the elementary solution of the associated scalar equation, which satisfies

$$\gamma * \dot{\mathscr{G}} - \nabla^2\mathscr{G} = \delta. \tag{15}$$

Incident fields are defined by the initial values $\mathbf{D}_0$ and $\mathbf{B}_0$ given in a homogeneous region, with no discontinuities at S, and they can be expressed by

$$\mathbf{E}^{\text{in}} = \mu_0\dot{\mathscr{G}} * \mathbf{D}_0\delta(t) + \nabla\mathscr{G} * \times\mathbf{B}_0\delta(t), \tag{16}$$

$$\mathbf{B}^{\text{in}} = \gamma * \mathscr{G} * \mathbf{B}_0\delta(t) - \mu_0\nabla\mathscr{G} * \times\mathbf{D}_0\delta(t). \tag{17}$$

The initial values $\mathbf{D}_0$ and $\mathbf{B}_0$ satisfy the constraints (1) and (2); that is, these fields are solenoidal. The incident fields are obtained from the initial conditions without solving any equations, essentially by integrations, and we consider them as known quantities. Fields $\mathscr{E}$ and $\mathscr{B}$ that vanish initially and have jumps $\boldsymbol{\phi} = \Delta\mathscr{E}$ and $\boldsymbol{\eta} = \Delta\mathscr{B}$ across S are given by

$$\begin{aligned}\mathscr{E} = &-\nabla\mathscr{G} * \hat{n}\cdot\boldsymbol{\phi}\delta(S) + \nabla\mathscr{G} * \times(\hat{n}\times\boldsymbol{\phi}\delta(S)) \\ &- \dot{\mathscr{G}} * \hat{n}\times\boldsymbol{\eta}\delta(S),\end{aligned} \tag{18}$$

$$\begin{aligned}\mathscr{B} = &-\nabla\mathscr{G} * \hat{n}\cdot\boldsymbol{\eta}\delta(S) + \nabla\mathscr{G} * \times(\hat{n}\times\boldsymbol{\eta}\delta(S)) \\ &+ \gamma * \mathscr{G} * \hat{n}\times\boldsymbol{\phi}\delta(S).\end{aligned} \tag{19}$$

Substitution into Eqs. (1), (2), (3), and (13) shows with the help of Eqs. (10) and (15) that the fields given by Eqs. (16)–(19) satisfy Maxwell's equations, provided that the jumps satisfy

$$\gamma_t * \hat{n}\cdot\boldsymbol{\phi} = -\nabla_S\cdot\hat{n}\times\boldsymbol{\eta}, \tag{20}$$

$$\hat{n}\cdot\dot{\boldsymbol{\eta}} = \nabla_S\cdot\hat{n}\times\boldsymbol{\phi}, \tag{21}$$

where γ_t and the convolution in Eq. (20) are restricted to the time variable. These last two equations determine the normal components of the jumps across S in terms of the tangential components when the jumps vanish initially; they are a consequence of Eqs. (3) and (13) when applied to the fields on both sides of S, and the surface divergence comes from the relation

$$\hat{n}\cdot\nabla\times\mathbf{u} = -\nabla_S\cdot(\hat{n}\times\mathbf{u}). \tag{22}$$

The general procedure to solve the scattering problem is the same one used for nondispersive media in Ref. 1.

Equations (18) and (19) are rewritten in the form

$$\mathscr{E} = \mathbf{L}\{\hat{n}\times\boldsymbol{\phi}\} + \mathbf{M}\{\hat{n}\times\boldsymbol{\eta}\}, \tag{23}$$

$$\mathscr{B} = \mathbf{L}\{\hat{n}\times\boldsymbol{\eta}\} + \mathbf{M}'\{\hat{n}\times\boldsymbol{\phi}\}; \tag{24}$$

that is, the fields, $\mathscr{E}$ and $\mathscr{B}$ are functionals of the tangential components of their jumps across S, as the normal components can be eliminated by means of Eqs. (20) and (21).

We define two sets of auxiliary fields that obey a single set of equations both in V_1 and V_2. The fields $\mathbf{E}_1$ and $\mathbf{B}_1$ are equal to the scattered fields in V_1 and obey the equations for the medium 1 also in V_2; the tangential component of $\mathbf{E}_1$ is continuous across S and the jump $\hat{n}\times\boldsymbol{\eta}$ in $\hat{n}\times\mathbf{B}_1$ is our one unknown tangential field. The fields $\mathbf{E}_2$ and $\mathbf{B}_2$ are equal to the transmitted fields in V_2 and vanish in V_1.

Equations (23) and (24) give

$$\mathbf{E}_1 = \mathbf{M}_1\{\hat{n}\times\boldsymbol{\eta}\}, \tag{25}$$

$$\mathbf{B}_1 = \mathbf{L}_1\{\hat{n}\times\boldsymbol{\eta}\}, \tag{26}$$

where the index on the functionals refer to the medium in V_1.

The jumps in $\hat{n}\times\mathbf{E}_2$ and $\hat{n}\times\mathbf{B}_2$ are equal to the boundary values of $\hat{n}\times\mathbf{E}$ and $\hat{n}\times\mathbf{B}$ in V_2, related to those in V_1 by the physical boundary conditions; that is, the continuity of $\hat{n}\times\mathbf{E}$ and $\hat{n}\times\mathbf{B}$ across S. Hence

$$\Delta(\hat{n}\times\mathbf{E}_2) = \hat{n}\times\mathbf{E}^{\text{in}} + \hat{n}\times\mathbf{E}_{1-}, \tag{27}$$

$$\Delta(\hat{n}\times\mathbf{B}_2) = \hat{n}\times\mathbf{B}^{\text{in}} + \hat{n}\times\mathbf{B}_{1-}, \tag{28}$$

where the subscript $1-$ refers to the boundary values of $\mathbf{E}_1$ and $\mathbf{B}_1$ in V_1. These jumps are thus determined by $\hat{n}\times\boldsymbol{\eta}$ via Eqs. (25) and (26), and we can write $\mathbf{E}_2$ and $\mathbf{B}_2$ in terms of $\hat{n}\times\boldsymbol{\eta}$ as

$$\mathbf{E}_2 = \mathbf{L}_2\{\Delta(\hat{n}\times\mathbf{E}_2)\} + \mathbf{M}_2\{\Delta(\hat{n}\times\mathbf{B}_2)\}, \tag{29}$$

$$\mathbf{B}_2 = \mathbf{L}_2\{\Delta(\hat{n}\times\mathbf{B}_2)\} + \mathbf{M}_2'\{\Delta(\hat{n}\times\mathbf{E}_2)\}. \tag{30}$$

We obtain the integral equation by imposing the condition that these fields vanish in V_1; in particular, we set

$$\hat{n}\times\mathbf{E}_{2-} = 0. \tag{31}$$

The precise forms of the functionals and integral equation depend on the properties of the medium, and we give some examples below.

III. ELEMENTARY SOLUTION OF THE SCALAR EQUATION

The solution of Eq. (15) is well known[4] for a simple dielectric, where $\sigma = 0$ and ϵ is independent of frequency; the result is usually written in the form

$$\mathscr{G}_0 = \delta(t - r/v)/(4\pi r), \tag{32}$$

where the speed of propagation of the wave is

$$v = (\epsilon\mu_0)^{-1/2}. \tag{33}$$

The support of this distribution is the forward light cone.

In general, the elementary solution depends on the properties of the medium. We can assume frequently that the elementary solution is a tempered distribution that has a Fourier transform $\mathscr{K}(\mathbf{k},\omega)$. Then Eq. (15) reduces to

$$[k^2 - (\omega^2/c^2)(1 + \chi_\omega + i\sigma_\omega/\epsilon_0\omega)]\mathscr{K}(\mathbf{k},\omega) = (2\pi)^{-2}, \tag{34}$$

where c is the speed of light in free space. The problem of finding the primitive of $\mathscr{K}$ with respect to the space variables gives the elementary solution of the Helmholtz equation, and we can write

$$\mathscr{G} = (1/2(2\pi)^{3/2}r)\mathscr{F}_-(e^{i\kappa r}), \tag{35}$$

where κ is the square root with the positive real part for positive ω of

$$\kappa^2 = \mu_0(\omega^2\epsilon_\omega + i\omega\sigma_\omega). \tag{36}$$

The distribution $\mathscr{G}$ will in general be singular, as we can see from the examples in Eq. (32) and others. These distributions can often be expressed as derivatives of functions, such as

$$\mathscr{G} = \frac{i}{2(2\pi)^{3/2}r}\frac{\partial}{\partial t}\mathscr{F}_-\left(\frac{e^{i\kappa r}}{\omega + i\epsilon}\right), \quad \epsilon \to 0+. \tag{37}$$

If $\kappa = \omega/v$, we obtain, in terms of the unit step function θ,

$$\mathscr{G}_0 = \frac{i}{2(2\pi)^{3/2}r}\frac{\partial}{\partial t}\left[-i(2\pi)^{1/2}\theta\left(t - \frac{r}{v}\right)\right], \tag{38}$$

which leads back to Eq. (32).

The relationship

$$\mathscr{F}_-[T(\omega + i\alpha)] = \exp(-\alpha t)\mathscr{F}_-[T(\omega)] \tag{39}$$

suggests that an imaginary term linear in ω in κ^2 as given by Eq. (36) leads to an overall damping factor, as can be seen in the case of the simple conductor.

The convolutions involving γ_t can be reduced to products of the Fourier transforms, where that of γ_t is (up to a factor $\sqrt{2\pi}$),

$$\gamma_\omega = \mu_0(-i\omega\epsilon_\omega + \sigma_\omega). \tag{40}$$

Thus, in principle, we can solve Eq. (20) for $\hat{n}\cdot\boldsymbol{\phi}$ if we write

$$\hat{n}\cdot\boldsymbol{\phi}(\mathbf{x},t) = \frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{\infty} d\omega\,\frac{\tilde{\eta}_\omega}{\gamma_\omega}e^{-i\omega t}, \tag{41}$$

where

$$\tilde{\eta}_\omega = \frac{1}{(2\pi)^{1/2}}\int_0^\infty dt\nabla_S\cdot\hat{n}\times\boldsymbol{\eta}(\mathbf{x},t)e^{i\omega t}. \tag{42}$$

The lower limit of the integral is 0 because $\boldsymbol{\eta}$ vanishes for negative times; we can thus assume that $\tilde{\eta}_\omega$ is analytic in the upper half of the ω-plane and tends to 0 as $\omega \to \infty$. The function $\hat{n}\cdot\boldsymbol{\phi}$ has the same properties as $\hat{n}\times\boldsymbol{\eta}$, which imposes restrictions on the form of γ_ω.

IV. THE SIMPLE CONDUCTOR

We consider in this section a medium that has constant permittivity and conductivity. Even when these quantities are independent of frequency, there is dispersion due to the losses in a conducting medium. The physical requirement that the effects of the medium become negligible in the high-frequency limit is not satisfied, but this approximation is good for slowly varying pulses and is relatively easy to study.

The resulting equation is known as the telegraphist's equation (A1), and the elementary solution is usually expressed in the form[5]

$$\begin{aligned}\mathscr{G}(\mathbf{x},t) = \exp\left(-\frac{\sigma t}{2\epsilon}\right)&\left\{\frac{\delta(t - r/v)}{4\pi r}\right.\\ &+ \frac{\sigma}{8\pi\epsilon v(t^2 - r^2/v^2)^{1/2}}\\ &\left.\times I_1\left[\frac{\sigma(t^2 - r^2/v^2)^{1/2}}{2\epsilon}\right]\theta\left(t - \frac{r}{v}\right)\right\},\end{aligned} \tag{43}$$

where I_1 is the modified Bessel function. In the Appendix we give a formal definition of this distribution and, following the procedure used in Ref. 6 for the wave equation, we show that it satisfies the telegraphist's equation. We also derive there the appropriate convolution products, which allow us to write the functionals in Eqs. (23) and (24) as

$$\begin{aligned}\mathbf{L}\{\hat{n}\times\boldsymbol{\phi}\} = \frac{1}{4\pi}\mathrm{P}\oint_S dS'\exp\left(-\frac{\sigma R}{2\epsilon v}\right)&\left[\hat{n}'\times\left(\frac{\dot{\boldsymbol{\phi}}_{\rm ret}}{v}\right.\right.\\ &\left.\left.+\frac{\sigma\boldsymbol{\phi}_{\rm ret}}{2\epsilon v} + \frac{\boldsymbol{\phi}_{\rm ret}}{R}\right)\right]\times\frac{\mathbf{R}}{R^2} + \nabla\times\mathbf{I}\{\hat{n}\times\boldsymbol{\phi}\},\end{aligned} \tag{44}$$

$$\begin{aligned}\mathbf{M}\{\hat{n}\times\boldsymbol{\eta}\} = \frac{1}{4\pi}\mathrm{P}\oint_S dS'\exp\left(-\frac{\sigma R}{2\epsilon v}\right)&\left[\hat{n}'\cdot\left(\frac{\dot{\boldsymbol{\phi}}_{\rm ret}}{v}\right.\right.\\ &\left.\left.+\frac{\sigma\boldsymbol{\phi}_{\rm ret}}{2\epsilon v} + \frac{\boldsymbol{\phi}_{\rm ret}}{R}\right)\frac{\mathbf{R}}{R^2} - \frac{\hat{n}'\times\dot{\boldsymbol{\eta}}_{\rm ret}}{R}\right]\\ &+\nabla I\{\hat{n}\cdot\boldsymbol{\phi}\} - \mathbf{I}\{\hat{n}\times\dot{\boldsymbol{\eta}}\},\end{aligned} \tag{45}$$

$$\begin{aligned}\mathbf{M}'\{\hat{n}\times\boldsymbol{\phi}\} = \frac{1}{4\pi}\mathrm{P}\oint_S dS'\exp\left(-\frac{\sigma R}{2\epsilon v}\right)&\left[\hat{n}'\cdot\left(\frac{\dot{\boldsymbol{\eta}}_{\rm ret}}{v}\right.\right.\\ &\left.\left.+\frac{\sigma\boldsymbol{\eta}_{\rm ret}}{2\epsilon v} + \frac{\boldsymbol{\eta}_{\rm ret}}{R}\right)\frac{\mathbf{R}}{R^2} + \frac{(\gamma_t * \hat{n}'\times\boldsymbol{\phi})_{\rm ret}}{R}\right]\\ &+\nabla I\{\hat{n}\cdot\boldsymbol{\eta}\} + \mathbf{I}\{\gamma_t * \hat{n}\times\boldsymbol{\phi}\},\end{aligned} \tag{46}$$

where the functional I comes from the second term in Eq. (A22) and is defined by

$$\begin{aligned}I\{\xi\} = \frac{\sigma}{8\pi\epsilon v}\oint_S dS'\int_{R/v}^\infty dt'\exp\left(-\frac{\sigma t'}{2\epsilon}\right)&\left(t'^2 - \frac{R^2}{v^2}\right)^{-1/2}\\ &\times I_1\left[\frac{\sigma(t'^2 - R^2/v^2)^{1/2}}{2\epsilon}\right]\xi(\mathbf{x}',t - t'),\end{aligned} \tag{47}$$

and $\mathbf{I}$ is obtained from I by replacing ξ by $\boldsymbol{\xi}$.

For the simple conductor, the convolution product in the time variable of the distribution γ_t as given by Eq. (14) and a surface field ξ is

$$\gamma_t * \xi = \mu_0\epsilon\dot{\xi} + \mu_0\sigma\xi. \tag{48}$$

We then can find $\hat{n}\cdot\boldsymbol{\phi}$ in terms of $\hat{n}\times\boldsymbol{\eta}$ from Eq. (20) and $\hat{n}\cdot\boldsymbol{\eta}$ in terms of $\hat{n}\times\boldsymbol{\phi}$ from Eq. (21) by integration; all of these fields vanish for $t\leqslant 0$.

The only terms in the integrands that become singular when the field point $\mathbf{x}$ is on the surface S are those that are proportional to $\mathbf{R}/R^3$, since the surface element has a factor R. The exponential factors become 1 when $R\to 0$, and the discontinuities of the fields are the same as those found for the simple dielectric; that is, the boundary values of the fields in V_1 and V_2 are related to the fields on the surface by

$$\mathscr{E}_{\pm} = \pm\tfrac{1}{2}\boldsymbol{\phi} + \mathscr{E}, \quad \mathbf{x}\in S, \tag{49}$$

$$\mathscr{B}_{\pm} = \pm\tfrac{1}{2}\boldsymbol{\eta} + \mathscr{B}, \quad \mathbf{x}\in S. \tag{50}$$

The solution of the scattering problem proceeds as outlined in Sec. III. In particular, the jumps in the fields $\hat{n}\times\mathbf{E}_2$ and $\hat{n}\times\mathbf{B}_2$ in Eqs. (27) and (28) are

$$\Delta\,(\hat{n}\times\mathbf{E}_2) = \hat{n}\times(\mathbf{E}^{\text{in}} + \mathbf{M}_1\{\hat{n}\times\boldsymbol{\eta}\}), \tag{51}$$

$$\Delta\,(\hat{n}\times\mathbf{B}_2) = \hat{n}\times(\mathbf{B}^{\text{in}} - \tfrac{1}{2}\boldsymbol{\eta} + \mathbf{L}_1\{\hat{n}\times\boldsymbol{\eta}\}), \tag{52}$$

and the integral equation (31) becomes

$$\hat{n}\times(\tfrac{1}{2}\mathbf{M}_1 - \mathbf{L}_2\mathbf{M}_1 + \tfrac{1}{2}\mathbf{M}_2 - \mathbf{M}_2\mathbf{L}_1)\{\hat{n}\times\boldsymbol{\eta}\} + \hat{n}\times(\tfrac{1}{2}\mathbf{E}^{\text{in}} - \mathbf{L}_2\{\hat{n}\times\mathbf{E}^{\text{in}}\} - \mathbf{M}_2\{\hat{n}\times\mathbf{B}^{\text{in}}\}) = 0, \tag{53}$$

which has the same form of that for the simple dielectric when we set to 1 the ratio α of the permeabilities of the two media. Once this equation is solved for $\hat{n}\times\boldsymbol{\eta}$ the scattered fields are given by (25) and (26), and the transmitted fields by (29) and (30).

V. THE COLLISIONLESS PLASMA

Another relatively simple example of a dispersive medium is that of a plasma that has a vanishing conductivity and a permittivity given by

$$\epsilon_\omega = \epsilon_0(1 - \omega_{\mathrm{p}}^2/\omega^2), \tag{54}$$

where ω_{p} is a constant called the plasma frequency. We substitute ϵ_ω into Eq. (36) and obtain

$$\kappa^2 = (1/c^2)(\omega^2 - \omega_{\mathrm{p}}^2). \tag{55}$$

The susceptibility $\chi_\omega = -\omega_{\mathrm{p}}^2/\omega^2$ tends to 0 as $\omega\to\infty$, and in the time domain we can write

$$\chi(t) = \omega_{\mathrm{p}}^2 t\theta(t), \tag{56}$$

whence

$$\gamma_t = \mu_0\epsilon_0[\delta'(t) + \omega_{\mathrm{p}}^2\theta(t)], \tag{57}$$

and the elementary solution $\mathscr{G}$ has to satisfy the equation

$$\frac{1}{c^2}\frac{\partial^2\mathscr{G}}{\partial t^2} - \nabla^2\mathscr{G} + \frac{\omega_{\mathrm{p}}^2}{c^2}\mathscr{G} = \delta. \tag{58}$$

The solution of this Klein–Gordon equation is given by[5]

$$\mathscr{G}(\mathbf{x},t) = \frac{\delta(t - r/c)}{4\pi r} - \frac{\omega_{\mathrm{p}}}{4\pi c(t^2 - r^2/c^2)^{1/2}} \times J_1[\omega_{\mathrm{p}}(t^2 - r^2/c^2)^{1/2}]\,\theta\Big(t - \frac{r}{c}\Big), \tag{59}$$

where J_1 is a Bessel function. The form of this elementary solution is essentially the same as that for the simple conductor without the exponential damping. The formulas in the Appendix and many of those in the previous section apply *mutatis mutandis*. For instance, the functional I becomes

$$I\{\xi\} = -\frac{\omega_{\mathrm{p}}}{4\pi c}\oint_S dS'\int_{R/v}^{\infty} dt' \times\frac{J_1[\omega_{\mathrm{p}}(t'^2 - R^2/c^2)^{1/2}]}{(t'^2 - R^2/c^2)^{1/2}}\xi(\mathbf{x}',t - t'). \tag{60}$$

The convolution product by Eq. (57) becomes

$$\gamma_t * \xi = \epsilon_0\mu_0\dot{\xi}(\mathbf{x},t) + \omega_{\mathrm{p}}^2\int_0^t dt'\,\xi(\mathbf{x},t'), \tag{61}$$

and we can solve Eq. (20) either via Eq. (41) or by solving the simple second-order differential equation

$$\mu_0\epsilon_0(\hat{n}\cdot\ddot{\boldsymbol{\phi}} + \omega_{\mathrm{p}}^2\hat{n}\cdot\boldsymbol{\phi}) = -\nabla_S\cdot\hat{n}\times\dot{\boldsymbol{\eta}}, \tag{62}$$

obtained from Eq. (20) by differentiation with respect to time.

VI. CONCLUDING REMARKS

We have shown that the formalism we developed in Ref. 1 for the scattering of electromagnetic waves by a simple dielectric body applies essentially unchanged to conducting and dispersive media. All of the calculations can be carried out in the time domain if the elementary solution of the scalar equation and the distributions ϵ and σ can be found explicitly from their Fourier transforms.

The examples of the simple conductor and the collisionless plasma discussed in Sec. IV and Sec. V show that, in addition to the functions of the retarded time evaluated at $\tau = t - R/v$, we have to carry out integrations over a range of arguments of the function from 0 to τ. The actual range may be reduced due to the damping factor for the conducting medium.

We have limited our discussion to electromagnetic fields, but the same ideas can be applied to other types of waves in dispersive media. Also, variations on the method presented here, such as the use of dyadic Green functions, lead to similar kinds of procedures.

Actually, any other theoretical or numerical solution of wave problems carried out in the time domain can in principle be extended to dispersive media without first going through the solution of the problem for a monochromatic field.

APPENDIX

The elementary solution of the telegraphist's equation satisfies

$$\mu_0(\epsilon\ddot{\mathscr{G}} + \sigma\dot{\mathscr{G}}) - \nabla^2\mathscr{G} = \delta. \tag{A1}$$

This solution is the distribution defined by

$$\langle\mathscr{G},\varphi\rangle = \int_0^\infty dt\, v^2 t\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\overline{\varphi}(vt,t) + \frac{\sigma^2}{4\epsilon^2 v}\int_0^\infty r^2\,dr\int_{r/v}^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\mathscr{I}(\zeta)\overline{\varphi}(r,t), \tag{A2}$$

where $v = (\epsilon\mu_0)^{-1/2}$, $\zeta = (\sigma/2\epsilon)(t^2 - r^2/v^2)^{1/2}$,

$$\mathscr{I}(\zeta) = I_1(\zeta)/\zeta, \tag{A3}$$

I_1 is the modified Bessel function, and $\overline{\varphi}$ is the average of the test function φ over a sphere of radius r; that is,

$$\overline{\varphi}(r,t) = \frac{1}{4\pi}\oint d\Omega\, \varphi(\mathbf{x},t). \tag{A4}$$

Differentiating with respect to t, we find

$$\overline{\frac{\partial\varphi}{\partial t}} = \frac{\partial\overline{\varphi}}{\partial t}, \quad \overline{\frac{\partial^2\varphi}{\partial t^2}} = \frac{\partial^2\overline{\varphi}}{\partial t^2}. \tag{A5}$$

We use Gauss's divergence theorem on a sphere of radius r to derive

$$\int_V dV\, \nabla^2\varphi = \oint_{S(r)} d\,\mathbf{S}\cdot\nabla\varphi, \tag{A6}$$

$$\int_0^r r^2\, dr \oint d\Omega\, \nabla^2\varphi = r^2\frac{\partial}{\partial r}\oint d\Omega\, \varphi, \tag{A7}$$

and, taking derivatives of both sides with respect to r, we conclude that

$$\overline{\nabla^2\varphi} = \nabla^2\overline{\varphi}. \tag{A8}$$

We now show that $\mathscr{G}$ satisfies Eq. (A1). We have

$$\begin{aligned} A &= \langle \mu_0(\epsilon\ddot{\mathscr{G}} + \sigma\dot{\mathscr{G}}) - \nabla^2\mathscr{G},\varphi\rangle \\ &= \langle \mathscr{G},\mu_0(\epsilon\ddot{\varphi} - \sigma\dot{\varphi}) - \nabla^2\varphi\rangle, \end{aligned} \tag{A9}$$

which, by Eqs. (A5) and (A8), becomes

$$\begin{aligned} A &= \int_0^\infty dt\, v^2 t \exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\Big[\mu_0\Big(\epsilon\frac{\partial^2\overline{\varphi}}{\partial t^2} \\ &\quad - \sigma\frac{\partial\overline{\varphi}}{\partial t}\Big) - \nabla^2\overline{\varphi}\Big]_{r=vt} \\ &\quad + \frac{\sigma^2}{4\epsilon^2 v}\int_0^\infty r^2\, dr\int_{r/v}^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\mathscr{I}(\zeta) \\ &\quad \times\Big[\mu_0\Big(\epsilon\frac{\partial^2\overline{\varphi}}{\partial t^2} - \sigma\frac{\partial\overline{\varphi}}{\partial t}\Big) - \nabla^2\overline{\varphi}\Big]. \end{aligned} \tag{A10}$$

We note that

$$\frac{\partial\overline{\varphi}(vt,t)}{\partial t} = \Big[v\frac{\partial\overline{\varphi}(r,t)}{\partial r} + \frac{\partial\overline{\varphi}(r,t)}{\partial t}\Big]_{r=vt}, \tag{A11}$$

$$\begin{aligned} &\frac{d}{dt}\Big[\frac{1}{v}\frac{\partial}{\partial t}(r\overline{\varphi}) - \frac{\partial}{\partial r}(r\overline{\varphi})\Big]_{r=vt} \\ &\quad = v^2 t\Big[\frac{1}{v^2}\frac{\partial^2\overline{\varphi}}{\partial t^2} - \nabla^2\overline{\varphi}\Big]_{r=vt}, \end{aligned} \tag{A12}$$

and integrate by parts to rewrite the first term in Eq. (A10)

$$\begin{aligned} A_1 &= \int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\frac{d}{dt}\Big[\frac{1}{v}\frac{\partial}{\partial t}(r\overline{\varphi}) - \frac{\partial}{\partial r}(r\overline{\varphi})\Big]_{r=vt} \\ &\quad - \mu_0\sigma v^2\int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)t\frac{\partial\overline{\varphi}}{\partial t}\Big|_{r=vt} \\ &= -\Big[\frac{1}{v}\frac{\partial}{\partial t}(r\overline{\varphi}) - \frac{\partial}{\partial r}(r\overline{\varphi})\Big]_{r=vt=0} \\ &\quad - \frac{\sigma}{2\epsilon}\int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\Big[t\frac{\partial\overline{\varphi}}{\partial t} + \overline{\varphi} + vt\frac{\partial\overline{\varphi}}{\partial r}\Big]_{r=vt} \\ &= \overline{\varphi}(0,0) - \frac{\sigma}{2\epsilon}\int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\Big[t\frac{d\overline{\varphi}(vt,t)}{dt} + \overline{\varphi}(vt,t)\Big] \\ &= \varphi(0,0) - \frac{\sigma^2}{4\epsilon^2}\int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)t\overline{\varphi}(vt,t). \end{aligned} \tag{A13}$$

We also integrate the second term in Eq. (A10) by parts to obtain

$$\begin{aligned} A_2 &= \frac{\sigma^2}{4\epsilon^2 v}\int_0^\infty r^2\, dr\int_{r/v}^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\overline{\varphi}(r,t)\Big[\frac{1}{v^2}\frac{\partial^2\mathscr{I}(\zeta)}{\partial t^2} \\ &\quad - \frac{\partial^2\mathscr{I}(\zeta)}{\partial r^2} - \frac{2}{r}\frac{\partial\mathscr{I}(\zeta)}{\partial r} - \frac{\sigma^2}{4\epsilon^2 v^2}\mathscr{I}(\zeta)\Big] \\ &\quad + \frac{\mu_0\sigma^2}{4\epsilon^2 v}\int_0^\infty r^2\, dr\exp\Big(-\frac{\sigma r}{2\epsilon v}\Big)\Big[\Big(\frac{\sigma}{2}\mathscr{I}(0) \\ &\quad + \epsilon\frac{\partial\mathscr{I}}{\partial t}\Big|_{\zeta=0}\Big)\overline{\varphi}\Big(r,\frac{r}{v}\Big) - \epsilon\mathscr{I}(0)\frac{\partial\overline{\varphi}}{\partial t}\Big|_{t=r/v}\Big] \\ &\quad + \frac{\sigma^2 v}{4\epsilon^2}\int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)t^2 \\ &\quad \times\Big[\frac{\partial\mathscr{I}}{\partial r}\Big|_{\zeta=0}\overline{\varphi}(vt,t) - \mathscr{I}(0)\frac{\partial\overline{\varphi}}{\partial r}\Big|_{r=vt}\Big] \\ &= \frac{\sigma^4}{16\epsilon^4 v^3}\int_0^\infty r^2\, dr\int_{r/v}^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\overline{\varphi}(r,t)\Big(\frac{d^2\mathscr{I}}{d\zeta^2} \\ &\quad + \frac{3}{\zeta}\frac{d\mathscr{I}}{d\zeta} - \mathscr{I}\Big) + \frac{\sigma^2 v}{8\epsilon^2}\int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)t^2 \\ &\quad \times\Big[\frac{1}{2}v\mu_0\sigma\overline{\varphi} - \Big(\frac{1}{v}\frac{\partial\overline{\varphi}}{\partial t} + \frac{\partial\overline{\varphi}}{\partial r}\Big)\Big]_{r=vt} \\ &= \frac{\sigma^2}{4\epsilon^2}\int_0^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)t\overline{\varphi}(vt,t), \end{aligned} \tag{A14}$$

where we have changed orders of integration and variables of integration, and we have used the properties of $\mathscr{I}(\zeta)$, derived from those of Bessel functions,

$$\mathscr{I}'' + (3/\zeta)\mathscr{I}' - \mathscr{I} = 0, \tag{A15}$$

$$\mathscr{I}(0) = \tfrac{1}{2}, \quad \mathscr{I}'(\zeta)/\zeta\,|_{\zeta=0} = \tfrac{1}{8}. \tag{A16}$$

Thus,

$$A = A_1 + A_2 = \varphi(0,0) = \langle\delta,\varphi\rangle, \tag{A17}$$

which concludes the proof.

To find the convolution products we rewrite Eq. (A2) in the form

$$\begin{aligned} \langle\mathscr{G},\varphi\rangle &= \int dV\frac{\varphi(\mathbf{x},r/v)}{4\pi r}\exp\Big(-\frac{\sigma r}{2\epsilon v}\Big) \\ &\quad + \frac{\sigma^2}{16\pi\epsilon^2 v}\int dV\int_{r/v}^\infty dt\exp\Big(-\frac{\sigma t}{2\epsilon}\Big)\mathscr{I}(\zeta)\varphi(\mathbf{x},t), \end{aligned} \tag{A18}$$

and recall that a singular distribution on a surface S is defined by

$$\langle\xi\delta(S),\varphi\rangle = \int_{-\infty}^\infty dt\oint_S dS\,\xi(\mathbf{x},t)\varphi(\mathbf{x},t). \tag{A19}$$

By the definition of the convolution of two distributions we have

$$\begin{aligned} &\langle\mathscr{G}*\xi\delta(S),\varphi\rangle \\ &\quad = \int dV'\frac{\exp(-\sigma r'/2\epsilon v)}{4\pi r'}\int_{-\infty}^\infty dt\oint_S dS\,\xi(\mathbf{x},t) \\ &\quad \times\varphi(\mathbf{x},\mathbf{x}'),t + r'/v) + \frac{\sigma^2}{16\pi\epsilon^2 v}\int dV'\int_{r'/v}^\infty dt' \\ &\quad \times\exp\Big(-\frac{\sigma t'}{2\epsilon}\Big)\mathscr{I}(\zeta)\int_{-\infty}^\infty dt\oint_S dS\,\xi(\mathbf{x},t) \\ &\quad \times\varphi(\mathbf{x} + \mathbf{x}',t + t'), \end{aligned} \tag{A20}$$

and we change variables of integration from $\mathbf{x}'$ and t to

$\mathbf{x}'' = \mathbf{x} + \mathbf{x}'$ and $t'' = t + t'$, where $t' = r'/v$ in the first term, to obtain

$$\langle \mathscr{G} * \xi\delta(S), \varphi \rangle = \int_{-\infty}^{\infty} dt'' \int dV'' \oint_S dS \frac{\exp(-\sigma|\mathbf{x}'' - \mathbf{x}|/2\epsilon v)}{4\pi|\mathbf{x}'' - \mathbf{x}|} \times \xi\left(\mathbf{x}'' - \mathbf{x}, t'' - \frac{|\mathbf{x}'' - \mathbf{x}|}{v}\right)\varphi(\mathbf{x}'', t'') + \frac{\sigma^2}{16\pi\epsilon^2 v}\int_{-\infty}^{\infty} dt'' \int dV'' \times \oint_S dS \int_{|\mathbf{x}'' - \mathbf{x}|/v}^{\infty} dt' \exp\left(-\frac{\sigma t'}{2\epsilon}\right)\mathscr{I}(\zeta) \times \xi(\mathbf{x}, t'' - t')\varphi(\mathbf{x}'', t''). \tag{A21}$$

We thus find that

$$\mathscr{G} * \xi\delta(S) = \oint_S dS' \frac{\exp(-\sigma R/2\epsilon v)\xi(\mathbf{x}', t - R/v)}{4\pi R} + \frac{\sigma^2}{16\pi\epsilon^2 v}\oint_S dS' \int_{R/v}^{\infty} dt' \times \exp\left(-\frac{\sigma t'}{2\epsilon}\right)\mathscr{I}(\zeta')\xi(\mathbf{x}', t - t'), \tag{A22}$$

where $\mathbf{R} = \mathbf{x} - \mathbf{x}'$, $R = |\mathbf{R}|$, and $\zeta' = (\sigma/2\epsilon) \times (t'^2 - R^2/v^2)^{1/2}$. The first term is the same one obtained for the wave equation with the addition of the exponential damping factor. If ξ vanishes for negative times, the time integration in the second term extends from R/v to t only and the same exponential damping term appears, which further limits the contributions to this integral.

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[3] E. Marx and D. Maystre, J. Math. Phys. **23**, 1047 (1982). We note that Eq. (A47) in this paper is missing a factor of $\sqrt{2\pi}$ on the right-hand side. We also recall that the convolution product is not necessarily defined for two arbitrary distributions.

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On the controllability of quantum-mechanical systems

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The systems-theoretic concept of controllability is elaborated for quantum-mechanical systems, sufficient conditions being sought under which the state vector ψ can be guided in time to a chosen point in the Hilbert space $\mathscr{H}$ of the system. The Schrödinger equation for a quantum object influenced by adjustable external fields provides a state-evolution equation which is linear in ψ and linear in the external controls (thus a bilinear control system). For such systems the existence of a dense analytic domain $\mathscr{D}_\omega$ in the sense of Nelson, together with the assumption that the Lie algebra associated with the system dynamics gives rise to a tangent space of constant finite dimension, permits the adaptation of the geometric approach developed for finite-dimensional bilinear and nonlinear control systems. Conditions are derived for global controllability on the intersection of $\mathscr{D}_\omega$ with a suitably defined finite-dimensional submanifold of the unit sphere $S_{\mathscr{H}}$ in $\mathscr{H}$. Several soluble examples are presented to illuminate the general theoretical results.

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I. INTRODUCTION

This paper is devoted to a formal investigation of the controllability of quantum-mechanical systems. Such a study is ultimately motivated by the importance, or potential importance, of precision methods for influencing the dynamical behavior of microsystems, in such diverse contexts as particle acceleration and detection, plasma physics, magnetic resonance, electron microscopy, modern solid-state technology, laser fusion, and optical communication. On the one hand, we may be interested in governing the time development of certain pertinent average quantities. More ambitiously, we may wish to guide the quantum state itself. It is this latter type of controllability which concerns us here.

A. Problem formulation

Consider a physical system whose state $\psi(t)$ evolves with time according to the law

$$\frac{d}{dt}\psi(t) = H_0\psi(t) + \sum_{l=1}^{r} u_l(t)H_l\psi(t), \quad \psi(0) = \psi_o, \qquad (1)$$

where ψ is a point in some abstract state space, $H_0,H_1,\ldots,H_r$ are operators in this space, and the $u_l(t)$ are time-dependent scalar control functions. For the case that $H_0,H_1,\ldots,H_r$ are linear operators, we say, in systems-theoretic parlance, that (1) is a *bilinear* system[1] since the last term is simultaneously linear in the state ψ and the controls u_l. The formulation (1) includes as a special case the dynamical law followed by a pure state in quantum theory, i.e., the Schrödinger equation

$$i\hbar\frac{d}{dt}\psi(t) = \left[H_0' + \sum_{l=1}^{r} u_l(t)H_l'\right]\psi(t), \qquad (2)$$

where $H_0',H_1',\ldots,H_r'$ are linear, Hermitian operators in the underlying state space $\mathscr{H}$ of the quantum-mechanical system and the u_l are real functions of t. The operator $H_0' \equiv i\hbar H_0$ is naturally interpreted as the Hamiltonian determining the free evolution of the quantum system, while the $u_lH_l' \equiv i\hbar u_lH_l$ represent its couplings or interactions with certain external agents. Through suitable adjustment of the c-number controls $u_l(t)$, these interactions may be used to guide the state $\psi(t)\in\mathscr{H}$.

One may also entertain *linear* control systems, such that none of the controls u_l appears in the same addend with the state ψ, as well as *nonlinear* systems of the form (1) but with one or more of the operators of $\{H_0,H_l\}$ nonlinear. However, these cases are of no immediate relevance to conventional quantum mechanics.

In general, the quantum-mechanical state space $\mathscr{H}$ is an infinite-dimensional Hilbert space. Although the H_l, if not H_0, could in principle depend on t, we shall confine our attention to the case that all these operators are time-independent. We further suppose that the u_l are piecewise-constant functions of t, the intervals of constancy being denoted $[t_i, t_{i+1})$, i integral. Under the stated conditions, the existence and uniqueness of a solution $\psi(t)$ between successive switching times t_i and t_{i+1} is guaranteed by the assumed quantum dynamics. During the prescribed interval, $H_0 + \Sigma_l u_l H_l$ is a constant, skew-Hermitian operator. Patently, there is associated with that operator a unique unitary operator $U(t, t_i)$, parametrized by t on $[t_i, t_{i+1})$, with the property $U(t, t_i)\psi(t_i) = \psi(t)$, where $U(t_i, t_i) = E$ (identity operator). One may therefore proceed to patch together the solutions for the separate intervals to obtain an acceptable, continuous solution $\psi(t)$, over the full range $t\in\mathbb{R}^+$.

Now, a differential system such as (1) is said to be *controllable* if, given two states ψ_o and ψ_f, there exists a time interval $[0,t_f]$ and a set of admissible controls $u_l(t)$ (in our case, piecewise-constant controls), such that the system trajectory beginning at $\psi(0) = \psi_o$ develops under the influence of $u(t)$ to arrive at $\psi(t_f) = \psi_f$. This concept has become one of the touchstones of mathematical systems theory,[2] a discipline deeply rooted in classical dynamics. It is our purpose to introduce the controllability concept into the quantum do-

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main and explore its limitations in that more fundamental setting.

B. Relevant prior work

In recent years substantial progress has been made, based in part on the seminal work of Chow,[3] toward understanding continuous-time finite-dimensional bilinear and (certain) nonlinear systems.[1,4–21] However, the quantum control problem is intrinsically infinite-dimensional. Thus the advances made in Refs. 1 and 4–21 cannot be applied directly to the problem of guiding quantum states—except in idealized situations where the state space becomes finite-dimensional (as when only spin degrees of freedom play a role).

Infinite-dimensional bilinear and nonlinear control systems have not been extensively investigated, although several pioneering efforts deserve note: (i) Both Koch[22] and Brockett[23] have addressed the problem of realization of infinite-dimensional bilinear systems. (ii) Stefan[24] has obtained results on local integrability of a special class of infinite-dimensional control systems. (iii) Ball and Slemrod[25] have established criteria for local stabilization of infinite-dimensional bilinear systems. (iv) Hermes[26,27] has determined sufficient conditions for local controllability of nonlinear delay and infinite-dimensional nonlinear systems.

To the authors' knowledge, very little has been published on the controllability of quantum systems *per se*. As a preliminary to the present work, Tarn, Huang, and Clark[28] have explored the formal basis for the modeling of quantum-mechanical control systems by appropriate Schrödinger equations. Earlier, Butkovskii and Samoilenko[29,30] discussed the control of quantum objects in broad terms and laid out a framework for further studies; a number of enlightening examples were treated, but mathematically definitive results were not presented. Recently, these last workers have announced general conditions for controllability of pure quantum states.[31] However, these findings must be viewed with some caution, since results for finite-dimensional bilinear systems were taken over from Refs. 11 and 12 without due attention to the domain problem for the relevant operators in Hilbert space.

C. Epitome of present approach

In the present contribution, we shall deal with the domain issue for the operators involved in quantum control—which are generally unbounded operators—by appealing to certain fundamental developments due to Nelson.[32,33] That is, we shall pursue our analysis with respect to an analytic domain of the Hilbert space: a dense domain invariant under the action of the given operators, on which the solution $\psi(t)$ of the Schrödinger equation can be expressed globally in exponential form. The existence of such a domain (in some interesting situations) is guaranteed by a theorem of Nelson. Against this underpinning, we are able to extend the geometric approach as implemented by Sussmann and Jurdjevic,[10,11] Krener,[14] Brockett,[16] Kunita,[19] and others (who are concerned only with bounded operators) to establish a series of global controllability conditions for the quantum case. It will be seen both formally and intuitively that, within the assumed framework based on piecewise-constant controls, global controllability on an *infinite*-dimensional submanifold of Hilbert space can never be attained in a practical sense: In general, a desired goal in the state space cannot be achieved with a finite number of manipulations of the control set $\{u_l(t)\}$. Accordingly, our detailed considerations regarding global control are narrowed to situations in which the Lie algebra $\mathscr{A}$ of the operators entering the quantum version of (1) yields a tangent space of constant, finite dimension.

Indeed, if we have to appeal to Nelson's theorem to assure the existence of an analytic domain, then we are already dealing with the following situation. The quantum system is one described by a finite-dimensional Lie group Γ, which is represented by unitary evolution operators on a Hilbert space $\mathscr{H}$. The control system—a bilinear system whose states are in $\mathscr{H}$—has the property that its associated Lie algebra is contained in the Lie algebra of operators on $\mathscr{H}$ obtained from the unitary representation of Γ. This specification is admittedly quite restrictive; therefore, it is not surprising that, with minimal attention to the infinite dimensionality of $\mathscr{H}$, we can bring to bear the techniques introduced for finite-dimensional manifolds in Refs. 10, 11, 14, 16, and 19. One may expect essential differences between finite-dimensional and infinite-dimensional problems to surface as one goes beyond the case of analytic vectors as initial conditions. The next step beyond analytic vectors and toward a less restrictive physical setting might involve "infinitely differentiable vectors"—those vectors of $\mathscr{H}$ for which the orbits are infinitely differentiable functions of the group parameters.

We hasten to point out that the above specification corresponding to Nelson's theorem does include the physical example of paramount importance in engineering applications, namely, the harmonic oscillator with coupling to external classical fields.

D. Organization of the paper

This paper is divided into six main sections. In Sec. II we collect certain key ideas and terminology from manifold theory and Lie algebra which are instrumental to our analysis of the control system (1) in infinite-dimensional space. Section III surveys the existing results on controllability for a finite-dimensional state space. In Sec. IV we introduce the concepts of analytic domain and analytic controllability, consider the implications of Nelson's theorem, and present arguments to the effect that, on an analytic domain, the controllability results obtained for a finite-dimensional state space can be extended to the quantum problem posed in Sec. IA. In Sec. V some examples are given to illustrate the concept of quantum controllability and the general findings of Sec. IV. We conclude, in Sec. VI, with a brief prospectus of outstanding problems in the largely unexplored intersection between quantum mechanics and mathematical systems theory.

II. MATHEMATICAL PRELIMINARIES

In general, the states of a quantum system are represented by vectors (or functions) in an infinite-dimensional space. With this in mind, we shall outline the essential manifold and Lie group theory appropriate to a Banach space. It is assumed that the reader has some familiarity with differentiable manifolds in the finite-dimensional context. In setting up the necessary catalog of concepts, we shall adhere closely to the conventions of Refs. 34–37.

A. Atlases and differentiable manifolds

As in the finite-dimensional case, the concept of *atlas* is introduced as a first step.[35,36] An atlas of a set M is again a collection of *charts* (U_i, φ_i), with $\cup_i U_i = M$. But now the bijective map φ_i is from the subset U_i of M onto some open subset of the *Banach space* $\mathscr{E}$, and for every pair i, j the set $\varphi_i(U_i \cap U_j)$ is open in $\mathscr{E}$. The atlas is said to be of class C^p if the mapping $\varphi_j \circ \varphi_i^{-1}$: $\varphi_i(U_i \cap U_j) \to \varphi_j(U_i \cap U_j)$ is of class C^p. (The cases "C^∞" and "analytic" are specified analogously.) For $\mu \in U_i \subset M$, the point $\varphi_i(\mu) \in \mathscr{E}$ is the *representative* of μ in the chart (U_i, φ_i).

The next step is to define a C^p *(-differentiable) manifold* modeled on $\mathscr{E}$, as a set M together with an equivalence class of C^p atlases modeled on $\mathscr{E}$. An equivalence relation is provided by the notion of *compatibility*: Two C^p atlases on M are compatible if their union is another such atlas. (To define C^∞-differentiable manifold and analytic manifold, proceed analogously.)

An example may be helpful at this point. Let the set M be $L^2(\mathbb{R}^n)$, let the U_i be open subsets of M with union equal to $L^2(\mathbb{R}^n)$, and let φ_i be the identity mapping. Then clearly M is a C^∞-differentiable and analytic manifold modeled on itself.

B. Tangent vectors, tangent bundles, and vector fields

Equivalent definitions[36] of *tangent vector* to M at point μ may be given (a) in terms of an equivalence class of curves and (b) in terms of the behavior of the representative of the object in question, under a change of charts.

Here we shall give explicit expression only to conception (a).

Definition: A parametrized curve γ on M is a mapping from $J \subset \mathbb{R}$ into M via $t \in J \to \gamma(t) \in M$.

Consider all differentiable curves γ: $J \subset \mathbb{R} \to M$ such that $\gamma(0) = \mu \in M$. We shall regard γ_1 as equivalent to γ_2 if in some chart (U, φ) (consequently,[35,36] in every chart) we have

$$\frac{d}{dt}(\varphi \circ \gamma_1)\Big|_{t=0} = \frac{d}{dt}(\varphi \circ \gamma_2)\Big|_{t=0}.$$

Definition: A *tangent vector* at μ to the manifold M, denoted $X\mu$ or $X(\mu)$, is defined by any one such equivalence class. The set of all such equivalence classes constitutes the *tangent-vector space* to M at μ, denoted $\mathscr{T}_\mu(M)$. The vector $v_\mu \equiv d(\varphi \circ \gamma)/dt\,|_{t=0}$ is termed the *representative*, in the chart (U, φ), of the vector tangent at μ to curve γ.

One may establish[35] that $\mathscr{T}_\mu(M)$ is isomorphic to $\mathscr{E}$ and accordingly has an intrinsic vector-space structure.

Definition: The *tangent fiber bundle* T(M) is given by $\cup_{\mu \in M} \mathscr{T}_\mu(M)$.

It is important to note[35,36] that T(M) has the structure of a differentiable manifold modeled on $\mathscr{E} \times \mathscr{E}$. Further, T(M) has a fiber bundle structure characterized by *base* M, *projection* π:$(\mu, X\mu) \to \mu$, *typical fiber* $\mathscr{E}$, and *structure group* $GL(\mathscr{E})$.

We are now equipped to formalize the idea of vector field for the case of an infinite-dimensional state space.[36]

Definition: A *vector field* X on a C^p (respectively, C^∞ or analytic) manifold M is a *cross section* of the tangent bundle T(M), by which we mean a class-C^{p-1} (respectively, class-C^∞ or analytic) mapping X: $M \to T(M)$, namely, X: $\mu \to (\mu, X\mu)$, such that $\pi \circ X$ is the identity.

C. Submanifolds, tangent subbundles, and integrability

Let M be a C^p manifold, $p \geqslant 0$, and consider a subset $N \subset M$ which still has C^p-manifold structure; then N will be called a *submanifold* of M. (The definition of a C^∞ or analytic submanifold runs parallel.) Between N and M there are some natural connections established by mappings (e.g., inclusive mappings). A thorough discussion is contained in Ref. 35. The tangent-vector space of N at μ is a subspace of $\mathscr{T}_\mu(M)$, the latter being, as we recall, an isomorphism of the Banach space $\mathscr{E}$. We can decompose $\mathscr{E}$ into Banach spaces $\mathscr{E}_1$ and $\mathscr{E}_2$ according to $\mathscr{E} = \mathscr{E}_1 \times \mathscr{E}_2$, where $\times$ indicates the Cartesian product and $\mathscr{T}_\mu(N)$ is an isomorphism of $\mathscr{E}_1$. The relationship of N to M can also be framed in terms of the tangent mappings[35,37] $\mathscr{T}_\mu i$: $\mathscr{T}_\mu(N) \to \mathscr{T}_\mu(M)$ and Ti: $T(N) \to T(M)$ induced by the inclusion i: $N \to M$.

Next there arises the notion of tangent subbundle (a subbundle of the tangent bundle over M). For details, see Refs. 35 and 36. A tangent subbundle corresponding to the submanifold N is specified in the same fashion as T(M), with N playing the role of M. But suppose, on the other hand, that we are *given* a tangent subbundle structure $S \subset T(M)$, and asked to determine whether or not there exists a submanifold—again call it N—which has tangent bundle S. This is the *integrability problem*. A simplified definition of integrability follows.

Definition: A tangent subbundle S over M is said to be *completely integrable*[38] at a point $\mu_0 \in M$ if there exists a submanifold N of M containing μ_0, such that the tangent map induced from the inclusion i: $N \to M$ has the property that for each $\nu \in N$, the tangent map $\mathscr{T}_\nu i$: $\mathscr{T}_\nu(N) \to \mathscr{T}_\nu(M)$ is a topologically linear isomorphism of $\mathscr{T}_\nu(N)$ on $\mathscr{S}_\nu(N)$.

We state a version of Frobenius' local existence theorem which gives conditions on S guaranteeing its integrability.[35]

Theorem 2.1 (Frobenius): With M and S respectively a manifold and tangent subbundle as above, S is integrable iff for each point $\mu \in M$ and all vector fields X and Y at μ which lie in S, the bracket $[X, Y]$ also lies in S. {It is to be understood here that X and Y are defined *on an open neighborhood of* μ. Also, in saying that X, for example, *lies in* S we mean that the image of each point μ of M under X lies in $\mathscr{S}_\mu(M)$. The bracket $[X, Y]$ is defined by $[X, Y](\nu) = X(Y(\nu)) - Y(X(\nu))$, where ν is any point in an open neighborhood of μ.} In other words, a necessary and sufficient condition for integrability of S is that its vector fields form a Lie algebra.

Definition[34]: The tangent subbundle S gives rise to a *regular foliation* of M if for any $\mu_0 \in M$ there is a submanifold N (called a *leaf* of the foliation corresponding to μ_0) whose tangent bundle coincides with S.

D. Flows; operations involving vector fields

We can formalize the idea of flow by direct extension of finite-dimensional geometry. Thus, we say that a vector field X has *flow* F_t if $dF_t(\mu)/dt = X(F_t(\mu))$, $\forall \mu \in \mathsf{M}$. If $F_t(\mu)$ is defined $\forall t \in \mathbb{R}$, we say X has a *complete* flow, and the vector field itself is termed complete. The local existence and uniqueness theorem for flows in the infinite-dimensional case of interest to us can be found in Ref. 37.

For the infinite-dimensional geometry one needs to define Lie derivative and Lie bracket without reference to local coordinates and their differentials. As in the finite-dimensional case, this may be done in terms of flows.[35,36] For example, the *Lie derivative* at time t of a function f: $\mathscr{E} \to \mathbb{R}^1$, with respect to the vector field X with flow F_s, is specified by

$$\pounds_X f = \lim_{s \to t} (s - t)^{-1} [f(F_s(\phi)) - f(F_t(\phi))] ,$$

where $\phi \in \mathscr{E}$. The Lie derivative $\pounds_X Y$ of a vector field Y with respect to X may be defined similarly.[35] With these definitions one can show[35] that if (as in Sec. IV) we work on an analytic domain,[32] the expressions $\pounds_X f = Xf$ and $\pounds_X Y = [X,Y]$, familiar from finite-dimensional theory, will apply. For nested commutators, it will be convenient to use the notation $\mathrm{ad}_X^j Y = [X, \mathrm{ad}_X^{j-1} Y]$, $j \geqslant 1$, with $\mathrm{ad}_X^0 Y = Y$.

E. Densely defined vector fields

To this point we have implicitly or explicitly assumed that various quantities such as vector fields, flows, curves, etc., are well-defined on some open subset of the Banach space. It is useful to consider extensions of these quantities which are "densely defined."[37]

Definition: A *manifold domain* $\mathsf{D} \subset \mathsf{M}$ is a dense subset D in a manifold M, such that (a) D is also a manifold and (b) the inclusion map i: $\mathsf{D} \to \mathsf{M}$ is smooth and $\mathsf{T}i$ has dense range.

Definition[37]: A *densely defined vector field* is a cross-section map X: $\mathsf{D} \to \mathsf{T}(\mathsf{M})$ such that $X(\rho) \in \mathscr{T}_\rho(\mathsf{M}) \forall \rho \in \mathsf{D}$. A *flow* (alternatively termed an integral curve) for X then consists of a collection of maps F_t: $\mathsf{D} \to \mathsf{D}$, $t \in \mathbb{R}$, with the properties (a) $F_{t+s}(\rho) = F_t \circ F_s(\rho)$ and $F_0(\rho) = \rho$, $\forall \rho \in \mathsf{D}$, and (b) $dF_t(\rho)/dt = X(F_t(\rho))$, $\forall \rho \in \mathsf{D}$, the derivative being evaluated considering $F_t(\rho)$ as a curve in M. If in the latter specification $t \in \mathbb{R}$ is replaced by $t \geqslant 0$, we speak of a *semiflow* (or a semiintegral curve).

It is easily seen that all the definitions, properties, and theorems quoted in this section, although designed for an infinite-dimensional state space, are also applicable if the dimensionality is finite.

III. CONTROLLABILITY IN FINITE-DIMENSIONAL SPACES

The purpose of this section is to present the relevant existing results on finite-dimensional control systems, in a form which allows their ready extension to the quantum control problem on an analytic domain.

A. Problem formulation and basic definitions

Consider a control system whose state vector m evolves on a real analytic manifold M according to the dynamical law

$$\frac{d}{dt} m(t) = X_0(m(t)) + \sum_{l=1}^{r} u_l(t) X_l(m(t)) . \tag{3}$$

Here $X_0, X_1, \ldots, X_r$ are (possibly nonlinear!) vector fields on M, which resides in a *finite*-dimensional space. The admissible class of control functions $u_l(t)$ (the set $\{u_1(t), \ldots, u_r(t)\}$ being abbreviated as u) is again chosen to be the class of piecewise-constant functions from $[0, \infty)$ into $\mathbb{R}$. For emphasis we have changed notation relative to formulation (1), which refers to the more general situation where the state space may be infinite-dimensional.

Let $\mathscr{V}(\mathsf{M})$ be the set of all real, analytic vector fields on M. By the Frobenius theorem of Sec. IIC, $\mathscr{V}(\mathsf{M})$ in fact constitutes a Lie algebra over the reals. Supposing $\mathfrak{S}$ is a subset of $\mathscr{V}(\mathsf{M})$ and $\mathscr{L}_1$ and $\mathscr{L}_2$ are Lie subalgebras of $\mathscr{V}(\mathsf{M})$, it will be useful to introduce the following sets:

$$\mathfrak{S}(m) \equiv \{ Y(m) | Y \in \mathfrak{S} \} ,$$

$$\{\mathfrak{S}\}_{\mathrm{LA}} \equiv \mathscr{L}(\mathfrak{S}) \equiv \text{Lie algebra generated by } \mathfrak{S}$$

$$\text{(smallest Lie subalgebra of } \mathscr{V}(\mathsf{M}) \text{ containing } \mathfrak{S}),$$

$$[\mathscr{L}_1, \mathscr{L}_2] \equiv \{ [X,Y] | X \in \mathscr{L}_1, \quad Y \in \mathscr{L}_2 \} .$$

Assume that the solutions of the differential equation (3) are defined for all $t \geqslant 0$, and denote an individual solution by $m(m_o, u, t)$, where m_o is the initial state vector and $u = \{u_l\}$. An important definition follows.

Definition: Given $m_o, m_f \in \mathsf{M}$, we say that m_f is *reachable* from m_o at time t if there exists an admissible control u such that $m_f = m(m_o, u, t)$. The *reachable set* from n at time t, i.e., the set of points in M reachable at t, is symbolized by $\mathsf{R}_t(n)$. In addition, we introduce the reachable set from n in positive time: $\mathsf{R}(n) \equiv \cup_{t>0} \mathsf{R}_t(n)$.

The task at hand is to characterize these reachable sets, which, of course, determine the extent to which the system is controllable. It is by now well known[10,11,16–19] that the structures of $\mathsf{R}_t(n)$ and $\mathsf{R}(n)$ are intimately related to the Lie algebras

$$\mathscr{A} \equiv \{ X_0, X_1, \ldots, X_r \}_{\mathrm{LA}} ,$$

$$\mathscr{B} \equiv \{ X_1, X_2, \ldots, X_r \}_{\mathrm{LA}} ,$$

$$\mathscr{C} \equiv \{ \mathrm{ad}_{X_0}^j X_l | l = 1, \ldots, r; j = 0, 1, \ldots \}_{\mathrm{LA}} .$$

The essential relations will be traced in the next subsection. We note that $\mathscr{A}$, $\mathscr{B}$, and $\mathscr{C}$ are not necessarily finite-dimensional.

It is appropriate at this juncture to identify the primary sources of the essential ideas and results of geometric control theory in the finite-dimensional case. The work of Chow[3] stands as an obvious pinnacle of the field. In the pre-Chow era, we may point to studies of Caratheodory[39,40] and Radon.[41] (References 40 and 41 contain material on the calculus of variations which bears implicitly on controllability.) Subsequent to Chow, the primary literature includes the work of Hermann,[4,42] Sussmann and Jurdjevic,[10,11] Krener,[14] and Stefan.[24] Among the other articles on finite-dimensional geometric control theory cited above, we have found Refs. 16 and 19 particularly useful in formulating our outline of the subject, which follows.

B. Basic results on controllability (finite-dimensional state space)

The analysis of control system (3) rests on four fundamental theorems: the theorem of Frobenius (cf. Sec. IIC), Chow's theorem,[3] and two theorems due to Sussmann and Jurdjevic.[10,11]

1. Frobenius' theorem is, of course, fundamental to the geometric analysis of the control system (3), as already indicated above. To be given the control system normally means to be given the X_k, $k = 0,1,...,r$, and the $u_l(t)$, $l = 1,...,r$. Hence the Lie algebra constructed from the X_k and their repeated commutators is available, and one can use the theorem to circumscribe the analytic manifold on which the system is destined to evolve—presuming such a manifold exists. If the vector fields of $\mathscr{A} = \{X_0,X_1,...X_r\}_{\rm LA}$ are complete, then the local existence property guaranteed by the theorem as stated in Sec. IIC can be given a global extension in the following sense[16]: There will exist a maximal submanifold N of M containing the arbitrarily specified point $m_o \in$M (or $\mu_o \in$M in the more general context of Sec. II), such that $\mathscr{A}(n)$ (respectively $\mathscr{A}(\nu)$) spans the tangent space of N at each point n (respectively ν) of N.

2. To show how Chow's theorem comes into the picture, we pursue a line of reasoning[16] which begins with the desire to quantify changes in the dynamics produced by changes of the control $u(t)$. How can we represent the actual effect of the control in terms of $X_0,X_1,...,X_r$ and $u(t)$? We can appeal to the Campbell–Baker–Hausdorff formula. Consider $X,Y\in\mathscr{V}$(M), and denote their flows by X_t, Y_t, respectively. Then

$$X_{t_1} \circ Y_{t_2}(m) = Z_t(m)|_{t=1}\ , \tag{4}$$

where

$$Z = t_1X + t_2Y + \tfrac{1}{2}t_1t_2[X,Y] + \cdots \tag{5}$$

is a formal series which converges for t_1 and t_2 both in some neighborhood of 0.

In terms of the Campbell–Baker–Hausdorff formula (4)–(5), we may readily appreciate the role played by the Lie algebra of $\{X_0,X_1,...,X_r\}$ in the controllability problem. Let us temporarily focus on the modified control system governed by the dynamical equation

$$\frac{d}{dt}m(t) = \sum_{k=0}^{r} u_k(t)X_k(m(t))\,, \tag{6}$$

where all the u_k are piecewise-constant real functions of time. [Note the presence of the extra control factor $u_0(t)$.] Again the Campbell–Baker–Hausdorff formula may be used to trace the dynamics, and we infer that if $X\in\{X_0,X_1,...,X_r\}_{\rm LA}$ then $X_t(m_o)$ (also denoted simply $X_t m_o$) belongs to the reachable set of the (modified) system.

On the other hand, we can enlist the following argument[16] to circumscribe the set of reachable points of system (6). Assume that the vector fields of $\mathscr{V}$(M) are complete, and consider an arbitrary member X of this set. Then, for each t a mapping X_t of M onto itself is provided by the flow on M corresponding to the differential equation $dm/dt = X(m)$. Consider the group diff(M) of diffeomorphisms of M, i.e., the set of all C^∞ one-to-one and onto mappings of this C^∞ manifold onto itself, such that the inverse mappings are likewise C^∞. Let the smallest subgroup of diff(M) which contains X_t for all X in $\{X_k|k = 0,1,...,r\}$ be symbolized by $\{\{X_k\}_t\}_{\rm G}$. Now, we can easily see that any point in M expressible as Wm_o, where $W\in\{\{X_k\}_t\}_{\rm G}$, can be reached from m_o along solution curves of (6). The indicated points are all like

$$(X_{\not k_0})_{t_0}(X_{\not k_1})_{t_1}\cdots(X_{\not k_r})_{t_r}m_o\ ,$$

where $\{\not k_0,\not k_1,...,\not k_r\} = \{0,1,...,r\}$; such points can certainly be attained by suitable switchings of the controls. One just sets $u_{\not k_r}\equiv 1$ and the $u_{k\neq \not k_r}\equiv 0$ for a time interval t_r, etc., finally setting $u_{\not k_0}\equiv 1$ and the $u_{k\neq\not k_0}\equiv 0$ for period t_0.

The obvious question is: How is the set of points $\mathsf{M}_1\equiv\{Wm_o\,|\,W\in\{\{X_k\}_t\}_{\rm G}\}$ related to the set $\mathsf{M}_2\equiv\{Lm_o|L\in\{\{L_i\}_t\}_{\rm G}\}$, where $\{L_i\} = \{X_k\}_{\rm LA} = \mathscr{A}$. We know that M_1 is reachable, while M_2 promises to be a larger set. It is here that Chow's theorem may be brought to bear; in effect, it says that the sets M_1 and M_2 are *identical* (under some modest conditions). We state the theorem in the version given by Brockett.[16]

Theorem 3.1 (Chow): Suppose that $\{X_0(m),X_1(m),...,X_r(m)\}$ is an assembly of vector fields such that the elements of the Lie algebra $\mathscr{A}(m) = \{X_0(m),X_1(m),...,X_r(m)\}_{\rm LA}$ are (a) C^∞ on a C^∞ manifold M with dim $\mathscr{A}(m)$ constant on M or (b) analytic on an analytic manifold M. Then, in either case, given any point $m_o\in$M, there exists a maximal submanifold M$'\subset$M containing m_o such that $\mathsf{M}_1 = \mathsf{M}_2 = \mathsf{M}'$. (*N.B.*: the arguments m are included in this statement to allow for the case that $X_0,X_1,...,X_r$ are nonlinear.)

We are thus able to draw some strong conclusions regarding the controllability of system (6) and the nature of its reachable set. But what about the system of immediate concern to us, namely (3)? Chow's theorem is not so incisive for this problem because it treats positive and negative times on an equal basis. The maximal submanifold M$'$ may contain points which can only be reached by moving *backwards* along the vector field $X_0(t)$. But in (3) there is no control factor $u_0(t)$ that we can set equal to -1, and such points are not actually reachable. Thus, in general, the reachable set R(m_o) for system (3) will be only a *proper subset* of the manifold M$' = \mathsf{M}_2$ characterized by the Lie algebra $\mathscr{A} = \{X_0,X_1,...,X_r\}_{\rm LA}$.

3. Against the background of Chow's theorem, some limited progress toward the characterization of the reachable set $\mathsf{R}_t(m_o)$ for system (3) has been made by Sussmann and Jurdjevic.[10,11] To present their results, we formally introduce the *maximal integral manifold* I$(\mathscr{W},m)$ of $\mathscr{W}$ passing through $m\in$M, where $\mathscr{W}$ is an arbitrary subalgebra of $\mathscr{V}$(M). Explicitly, we mean by this that I$(\mathscr{W},m)$ is the largest connected submanifold N of M which contains m and has the property that for all $n\in$N, the tangent space to N at n is $\mathscr{W}(n)$. The existence of I$(\mathscr{W},m)$ follows from the global version of Frobenius' theorem. We also introduce, for $t>0$, $\mathsf{I}_t(\mathscr{W},m) \equiv \mathsf{I}(\mathscr{W},X_{0t}(m))$. The relevant theorems are then:

Theorem 3.2 (Sussmann and Jurdjevic[10]): Let X_t and Y_t denote, respectively, the one-parameter flows of the vector fields $X,Y\in\mathscr{A}$. Then for all $m\in$M and $t\in\mathbb{R}$, $X_t(\mathsf{I}(\mathscr{C},m)) = Y_t(\mathsf{I}(\mathscr{C},m))$. In particular, $X_{0t}(\mathsf{I}(\mathscr{C},m))$ is the unique maximal integral manifold of $\mathscr{C}$ through $X_{0t}(m)$. (*N.B.*: the definitions of Lie algebras $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$ given in Sec. IIIA.)

Theorem 3.3 (Sussmann and Jurdjevic[10,17]): For all $m \in \mathsf{M}$ and $t > 0$, the reachable set $\mathsf{R}_t(m)$ of system (3) is a subset of $\mathsf{I}_t(\mathscr{C}, m)$; moreover, with respect to the topology of $\mathsf{I}_t(\mathscr{C}, m)$, the set $\mathsf{R}_t(m)$ is contained in the closure of its own interior.

The latter theorem tells us that $\mathsf{R}_t(m)$ has a nonempty interior in $\mathsf{I}_t(\mathscr{C}, m)$. This result ensues from the decomposition $\mathscr{A} \supset \mathscr{C} \supset \mathscr{B}$ of $\mathscr{A}$.

4. We are now equipped with the basic tools needed to pursue the controllability problem for system (3).

Definition: System (3) is said to be *strongly completely controllable* if $\mathsf{R}_t(m) = \mathsf{M}$ holds for all $t > 0$ and all $m \in \mathsf{M}$. If $\mathsf{R}(m) = \mathsf{M}$ holds for all m, the system is called *completely controllable*.

Following Kunita,[19] the key controllability results for our system will be framed in terms of families of vector fields drawn from $\mathscr{V}(\mathsf{M})$. In so doing, we make use of the following classification of vector fields, or more directly their associated integral curves.

Definition: With $m \in \mathsf{M}$, the integral curve $\{X_s(m), s \in \mathbb{R}\}$ is *attainable* [by system (3)] if both $X_t(m)$ and $X_{-t}(m)$ belong to $c\ell \mathsf{R}_t(m)$ for any $t > 0$ up to the closure time. If $X_t(m)$, but not necessarily $X_{-t}(m)$, belongs to $c\ell \mathsf{R}_t(m)$, we speak of *semiattainability*. On the other hand, if the more stringent condition is met that the full curve $\{X_s(m), s \in \mathbb{R}\}$ belongs to $c\ell \mathsf{R}_t(m)$, again for any $t > 0$, we say that $\{X_s(m), s \in \mathbb{R}\}$ is *strongly attainable*. *Strong semiattainability* of $\{X_s(m), s \in \mathbb{R}\}$ applies when the half curve $\{X_s(m), s \in \mathbb{R}^+\}$ belongs to $c\ell \mathsf{R}_t(m)$, $\forall t > 0$. The set of all vector fields on M whose integral curves are attainable (respectively, strongly attainable) is denoted by $\mathfrak{A}$ (respectively, $\mathfrak{A}_S$). The notation $\mathfrak{A}^+$ (respectively, $\mathfrak{A}_S^+$) is used for the corresponding semiattainable (respectively, strong semiattainable) case.

The above nomenclature is rooted in the nature of control systems, being manifestly predicated on the structure of the state-evolution equation, and in particular on what constraints are imposed on the control factors attached to $X_0, X_1, \ldots, X_r$. For example, set the u_l, $l = 1, \ldots, r$, identically zero and consider the autonomous system $dX_t/dt = X_0(X_t)$. It is seen that X_0 belongs to $\mathfrak{A}^+$ but not to $\mathfrak{A}$, since only one direction, and no control of amplitude, is associated with this vector field (i.e., $u_0 \equiv 1$). Now consider instead the system (3) with $X_0 \equiv 0$, thus the evolution equation $dm(t)/dt = \Sigma_{l=1}^r u_l X_l(m(t))$, and suppose the controls are restricted by $|u_l| = 1$ or 0. In this case we see that the vector fields $X_1, \ldots, X_r$ belong to $\mathfrak{A}$ because their effect on the dynamical state can be directed by $u_1, \ldots, u_r$; however, $X_1, \ldots, X_r \notin \mathfrak{A}_S$ because the amplitudes with which these vector fields enter the dynamical law cannot be manipulated with sufficient flexibility. On the other hand, when *no* constraints are imposed on the u_l, $l = 1, \ldots, r$ (apart from piecewise constancy), it is clear that $\mathscr{B} = \mathscr{L}(X_1, \ldots, X_r) \subset \mathfrak{A}_S$. For then $X_1, \ldots, X_r$ can always be "scaled" by appropriate controls $u_1(t), \ldots, u_r(t)$ in such a way that $m(t)$ reaches, at any chosen time t_f, any selected point on the manifold characterized, through the global version of Frobenius' theorem, by $\mathscr{B}$.

Besides the concept of attainable, semi-attainable, etc. sets, it is convenient to introduce the following notation. Let $\mathfrak{B}$ be a subset of $\mathscr{V}(\mathsf{M})$ and X an element of $\mathscr{V}(\mathsf{M})$. For a given positive integer q, consider the set of vector fields $\mathrm{ad}_{X^{(1)}}^{i_1} \cdots \mathrm{ad}_{X^{(p)}}^{i_p} X$ such that $i_1 + \cdots + i_p = q$, where $X^{(1)}, \ldots, X^{(p)}$ are mutually commuting, complete vector fields belonging to $\mathfrak{B}$. Denote the collection of *all* vector fields constructed in this manner, allowing for all qualifying choices of $\{X^{(1)}, \ldots, X^{(p)}\}$ in $\mathfrak{B}$, where p is to be varied also, by $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$. The subset of $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$ such that at least one of the indices $i_1, \ldots, i_p$ is odd, will be designated odd $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$. [The basic reason we are interested in odd $\mathrm{ad}_{\mathfrak{B}}^{(q)} X$ is that it belongs to $\mathfrak{A}_S$, provided $X \in \mathfrak{A}^+$ and $X^{(1)}, \ldots, X^{(p)} \in \mathfrak{A}_S$ (Ref. 19).]

Two important theorems on the controllability of system (3) may now be established. Proofs are given in Refs. 19 and 43. It is assumed that $\dim \mathsf{M} = d < \infty$.

Theorem 3.4 (Kunita[19]): (i) If $\dim \mathfrak{A}_S(m) = d$ holds for all $m \in \mathsf{M}$, then system (3) is strongly completely controllable. (*N.B.*: $\mathfrak{A}_S$ is a Lie algebra.)

(ii) If $\dim \mathscr{L}(\mathfrak{A})(m) = d$ holds for all $m \in \mathsf{M}$, then system (3) is completely controllable.

Theorem 3.5 (Kunita[19]): Assume that for control system (3) one can find a sequence of sets $\mathfrak{B}_j$ of vector fields, $j = 0, 1, 2, \ldots$, with ordering $\mathfrak{B}_0 \subset \mathfrak{B}_1 \subset \mathfrak{B}_2 \subset \cdots$, which meet the following two criteria:

(i) $\mathfrak{B}_0 \subset \mathscr{B} = \mathscr{L}(X_1, \ldots, X_r)$;

(ii) for each value of the index j there exists a positive integer q_j such that $\mathrm{ad}_{\mathfrak{B}_j}^{(q_j+1)} X_0 \subset \mathscr{L}(\mathfrak{B}_j)$ and $\mathfrak{B}_{j+1} \subset \mathscr{L}(\mathfrak{B}_j$, odd $\mathrm{ad}_{\mathfrak{B}_j}^{(q_j)} X_0)$. It follows that $\mathscr{L}(\cup_{j=0}^{\infty} \mathfrak{B}_j) \subset \mathfrak{A}_S$. If in fact $\dim \mathscr{L}(\cup_{j=0}^{\infty} \mathfrak{B}_j)(m) = d$ holds for all $m \in \mathsf{M}$, system (3) is strongly completely controllable on M.

Corollary 3.5.1 (Kunita[19]): If $\dim \mathscr{C}(m) = d$ holds for all $m \in \mathsf{M}$ and $[\mathscr{C}, \mathscr{B}] \subset \mathscr{B}$, system (3) is strongly completely controllable.

These last two theorems summarize the main results from finite-dimensional control theory which we would like to extend to quantum dynamics. However, such extensions—to the extent that they are possible—necessitate careful attention to the domain problem arising from the infinite dimensionality of the quantum state space.

IV. CONTROLLABILITY OF QUANTUM-MECHANICAL SYSTEMS

Let us return now to the quantum-mechanical control problem formulated in Sec. I. Since in this case $H_0, H_1, \ldots, H_r$ of (1) must be linear, skew-Hermitian operators on a Hilbert space $\mathscr{H}$ and the $u_l(t)$ are piecewise-constant by assumption, there will be associated, with the quantum dynamics, a Lie group Γ whose elements may be represented by unitary operators on $\mathscr{H}$. The usual statistical interpretation of the state vector (wave function) $\psi(t)$ is reflected in its unitary evolution. The scalar product of vectors ϕ_1, ϕ_2 in the Hilbert space $\mathscr{H}$ is denoted $\langle \phi_1 | \phi_2 \rangle$. Imposing unit norm at the initial time $t = 0$, we have $\langle \psi(t) | \psi(t) \rangle = 1$ $\forall t$; i.e., the dynamics unfold on the unit sphere of $\mathscr{H}$, denoted $\mathsf{S}_{\mathscr{H}}$.

A geometric description of quantum dynamics paralleling the description of Sec. III is facilitated by treating the state space $\mathscr{H}$ of the quantum system as a *real* Hilbert space. To this end, we may assert the formal decomposition

$\mathscr{H} = \mathscr{H}^R \times \mathscr{H}^I$, where $\mathscr{H}^R$ and $\mathscr{H}^I$ are real Hilbert spaces, isomorphic to one another. This decomposition is given meaning as follows. Consider an arbitrary state vector ϕ, interpreted to begin with as a vector in complex Hilbert space. We may choose some representation and identify real and imaginary parts, $\phi = \phi^R + i\phi^I$. Then ϕ^R is assigned to the space $\mathscr{H}^R$, i.e., $\phi^R \in \mathscr{H}^R$, while ϕ^I is assigned to $\mathscr{H}^I$. Thus ϕ is reinterpreted as a vector in a real Hilbert space constructed as the Cartesian product of $\mathscr{H}^R$ and $\mathscr{H}^I$. Correspondingly, we agree to compute the scalar product $\langle \phi_1 | \phi_2 \rangle$ as

$$\langle \phi_1 | \phi_2 \rangle = \langle \phi_1^R, \phi_2^R \rangle + \langle \phi_1^I, \phi_2^I \rangle ,$$

where $\langle \phi_1^R, \phi_2^R \rangle$ (respectively, $\langle \phi_1^I, \phi_2^I \rangle$) is the usual scalar product in the real Hilbert space $\mathscr{H}^R$ (respectively, $\mathscr{H}^I$). Since, in this work, we shall never have occasion to ascribe physical significance to the scalar product of two different vectors, these conventions will not bring us into conflict with those ordinarily adopted in quantum theory.[44] (For norms of state vectors, the two views obviously coincide.)

The above formal reinterpretation of $\mathscr{H}$, while entailing no loss of generality within the context of our aims, allows us to endow certain subsets of $\mathscr{H}$ with manifold structure. In particular, $S_{\mathscr{H}}$ is an infinite-dimensional submanifold of $\mathscr{H}$. For an explicit verification of the manifold character of $S_{\mathscr{H}}$, see Lang,[35] pp. 28–29. To see the geometric structure of $S_{\mathscr{H}}$, choose the local chart around $\chi_i \in S_{\mathscr{H}}$ as the projection of a neighborhood $U_i(\chi_i)$ to the space $\mathscr{H}_i \equiv \{ \eta | \langle \eta | \chi_i \rangle = 0, \eta \in \mathscr{H} \}$. The latter is manifestly a closed infinite-dimensional subspace of $\mathscr{H}$; moreover, $\mathscr{H}_i$ is isomorphic to $\mathscr{H}_j$ for all $\chi_i, \chi_j \in S_{\mathscr{H}}$.

A prominent feature of the quantum problem is that $H_0, H_1, ..., H_r$ are generally unbounded operators; it then becomes important to bring into play the notions of densely defined vector fields, and associated flows, curves, etc., introduced in Sec. II.

In this section, it is our primary task to show how results on controllability of finite-dimensional control systems, surveyed in Sec. III, can be generalized to infinite-dimensional, quantum-mechanical systems by exploitation of the properties of a certain type of manifold domain—an *analytic domain* $\mathscr{D}_\omega$. The existence of such a domain is assured by Nelson's theorem,[32] for a restricted but nontrivial class of skew-Hermitian operators $H_0, H_1, ..., H_r$. The conditions entering this theorem will appear rather restrictive, since they imply in particular that the Lie algebra $\mathscr{A} = \mathscr{L}(H_0, H_1, ..., H_r)$ associated with the quantum control system (1)–(2) is *contained* in the Lie algebra of operators on $\mathscr{H}$ obtained from the unitary representation of Γ. Still, the case of greatest relevance to engineering applications is included, namely, the harmonic oscillator with couplings to external classical fields. Moreover, an alternative formulation may be considered in which Nelson's theorem is not invoked: If one simply *assumes* the existence of an analytic domain $\mathscr{D}_\omega$, the extensions go through provided only that one imposes the additional assumption that the tangent space defined by $\mathscr{A}(\zeta)$ has constant finite dimension for all $\zeta \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$. Within such a formulation the possibility remains open (at this point) that the Lie algebra $\mathscr{A}$ produced by $H_0, H_1, ..., H_r$ is *larger* than that derived from the group Γ, conceivably infinite-dimensional.

In either formulation, the problem of practical interest will of necessity be one of controllability on a *finite-dimensional* submanifold of the infinite-dimensional manifold $S_{\mathscr{H}}$ available to the normalized quantum state. This limitation of our treatment will be explained in Sec. IVC; in brief, controllability on $S_{\mathscr{H}}$ would entail infinite sequences of switchings of the $u_l(t)$.

A. Analytic vector and analytic domain

The reader should consult the original work of Nelson[32] for the underlying motivation and detailed development of the concepts of analytic vector and analytic domain (see also Ref. 33). In the interests of logical completeness, we should, nevertheless, recall the definition of analytic vector.

Definition: Let A be an operator in $\mathscr{H}$. An element ω of $\mathscr{H}$ is called an *analytic vector* for A if the series expansion of $(\exp sA)\omega$ has a positive radius of convergence, that is, if

$$\sum_{n=0}^{\infty} \frac{\|A^n \omega\|}{n!} s^n < \infty$$

for some real $s > 0$, where $\|A^n \omega\|$ is the Hilbert-space norm of $A^n \omega$.

Note that if A is bounded, all vectors of $\mathscr{H}$ are trivially analytic vectors for A; i.e., the concept of analytic vector becomes an incisive one only when dealing with unbounded operators—which, of course, are prevalent in quantum mechanics.

We should also state what it means to be an analytic vector for a Lie algebra.

Definition: A vector ω qualifies as an *analytic vector* for a Lie algebra $\mathscr{L}$ if for some $s > 0$ and some basis of the Lie algebra, say $\{H_{(1)}, ..., H_{(d)}\}$, the series

$$\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\substack{1 \leqslant i_1 < \cdots < i_d \leqslant d \\ n_1 + \cdots + n_d = n}} \|H_{(i_1)}^{n_1} \cdots H_{(i_d)}^{n_d} \omega\| s^n$$

converges.

The theorem of Nelson which is relevant to the present investigation is:

Theorem 4.1 (Nelson[32]): Let $\mathscr{L}$ be a Lie algebra of skew-Hermitian operators in a Hilbert space $\mathscr{H}$, the operator basis $\{H_{(1)}, ..., H_{(d)}\}$, $d < \infty$, of $\mathscr{L}$ having a common invariant dense domain. If the operator $T = H_{(1)}^2 + \cdots + H_{(d)}^2$ is essentially self-adjoint, then there exists a unitary group Γ on $\mathscr{H}$ with Lie algebra $\mathscr{L}$. Let $\overline{T}$ denote the unique self-adjoint extension of T. Then it furthermore follows that the analytic vectors of $\overline{T}$ (i) are analytic vectors for the whole Lie algebra $\mathscr{L}$ and (ii) form a set invariant under Γ and dense in $\mathscr{H}$.

The vital implication of this theorem for our work is that it establishes the existence, under definite conditions, of a dense domain $\mathscr{D}_\omega$ of analytic vectors which provides a foothold for the extension of the controllability results of Sec. III to the quantum problem (1)–(2). Indeed, the set of analytic vectors of $\overline{T}$ will constitute such a subspace $\mathscr{D}_\omega$ of $\mathscr{H}$. Making the obvious identification $\mathscr{L} = \mathscr{A}$, the elements of $\mathscr{A}$ are then seen to be densely defined vector fields on $\mathscr{D}_\omega \cap \mathsf{M}$, where M is a finite-dimensional manifold on which the system point evolves with time. (Such a manifold surely exists under the prevailing assumptions; we could, for example, choose it to be the manifold characterized by $\mathscr{A} = \{H_0, H_1, ..., H_r\}_{\mathrm{LA}}$ through Frobenius' theorem.) We also have the corresponding "densely defined" flows (cf. Sec. IIE).

The detailed reasoning runs as follows. Under the provisions of Nelson's theorem and by the nature of analytic vectors, we know that any element of the unitary group Γ associated with $\{H_0, H_1, ..., H_r\}$ can be represented locally in the exponential form $\exp Xt$, where X is some element of $\mathscr{A}$. Moreover, this exponential expression can be extended globally in t (see Refs. 32 and 33); in other words, if the elements of $\mathscr{A}$ are vector fields, they are in fact complete. That the elements of $\mathscr{A}$ do qualify as vector fields can be seen in terms of the definition given in Sec. IIB. First, $\gamma = (\exp Xt)\psi_o$ is a parametrized curve on manifold M with $\gamma(0) = \psi_o \in \mathsf{M}$. Hence $d(\varphi \circ \gamma)/dt\,|_{t=0}$ represents a tangent vector; choosing for φ the identity mapping, $X\psi_o$ represents a tangent vector at ψ_o on M. If, in particular, $\dim \mathscr{A}(\zeta) = \dim(\mathsf{M} \cap \mathscr{D}_\omega) = d < \infty$, $\forall \zeta \in \mathsf{M} \cap \mathscr{D}_\omega$, then it is sufficient to use $\mathscr{A}$ to characterize the tangent space $\mathscr{T}_\zeta(\mathsf{M})$ to M at ζ, and the tangent bundle $\mathsf{T}(\mathsf{M}) = \cup_{\zeta \in \mathsf{M} \cap \mathscr{D}_\omega} \mathscr{T}_\zeta(\mathsf{M})$. Referring now to the definition of vector field (and the definition of densely defined vector field, Sec. IIE), the elements X of $\mathscr{A}$ assuredly qualify as (densely defined) vector fields, since we may associate with each a mapping X: $\mathsf{M} \cap \mathscr{D}_\omega \to \mathsf{T}(\mathsf{M})$, with $X(\zeta) = (\zeta, X\zeta)$, $\zeta \in \mathsf{M} \cap \mathscr{D}_\omega$. In fact, each X is an *analytic vector* field on $\mathsf{M} \cap \mathscr{D}_\omega$ since φ is taken as the identity.

B. Analytic controllability

With an analytic domain at our disposal, it is advantageous to modify the notion of controllability, as follows.

Definition: Assuming that an analytic domain exists, system (1)–(2) is called *strongly analytically controllable* on $\mathsf{M} \subseteq \mathsf{S}_{\mathscr{H}}$ if $\mathsf{R}_t(\zeta) = \mathsf{M} \cap \mathscr{D}_\omega$ holds for all $t > 0$ and all $\zeta \in \mathsf{M} \cap \mathscr{D}_\omega$. If $\mathsf{R}(\zeta) = \mathsf{M} \cap \mathscr{D}_\omega$ holds for all $\zeta \in \mathsf{M} \cap \mathscr{D}_\omega$, the system is termed *analytically controllable on* M.

Within the formulation set up in Sec. IVA, in which we appeal to Nelson's theorem, we can choose M as the closure of the set $\{e^{s_0 H_0} e^{s_1 H_1} \cdots e^{s_r H_r} \psi_o,\ s_k \in \mathbb{R},\ k = 0,1,...,r\}$; this is certainly the maximal manifold on which the system will evolve from $\psi_o \in \mathsf{M} \cap \mathscr{D}_\omega$. From previous considerations we know that M is necessarily a finite-dimensional submanifold of $\mathsf{S}_{\mathscr{H}}$, that $H_0, H_1, ..., H_r$ are densely defined vector fields on $\mathsf{M} \cap \mathscr{D}_\omega$, which is, of course, dense in M, and that the tangent space of $\mathsf{M} \cap \mathscr{D}_\omega$ at ζ is characterized by $\mathscr{A}(\zeta)$, $\forall \zeta \in \mathsf{M} \cap \mathscr{D}_\omega$. If $\mathscr{A}(\chi)$ is of dimension d, for all $\chi \in \mathsf{S}_{\mathscr{H}} \cap \mathscr{D}_\omega$, we see that $\mathsf{S}_{\mathscr{H}}$ has been partitioned into a foliation with d-dimensional regular manifolds as leaves.

We are now ready to pursue the question of analytic controllability on M, in analogy with the treatment of Sec. III. On $\mathsf{M} \cap \mathscr{D}_\omega$, the flows of vector fields of $\mathscr{A}$ take exponential form, by virtue of the properties of an analytic domain. Hence a Taylor expansion is always well defined for any such flow. Consequently, the *Campbell–Baker–Hausdorff* formula applies, making available computational techniques which parallel those employed for the finite-dimensional state space. (The only distinction is that the norm is now calculated in Hilbert space.) At the same time, the *Frobenius theorem* stated in Sec. IIC is also valid with respect to $\mathscr{D}_\omega$, i.e., with M replaced by $\mathsf{M} \cap \mathscr{D}_\omega$. What about Chow's theorem? In the general infinite-dimensional case, the validity of this theorem is questionable. To see that it may be carried over to the present context, consider that the proof of the theorem (see, for example, Refs. 10 and 11) is based on (i) a paracompact topology for the manifold in question (here, $\mathsf{M} \cap \mathscr{D}_\omega$), (ii) finite dimensionality of the tangent space of that manifold, and (iii) the Campbell–Baker–Hausdorff formula. We have already seen that it is legitimate to invoke (iii), while it is well known that the submanifolds of a normed topological space (like $\mathscr{H}$) are always paracompact with respect to the relative topology. The crucial prerequisite is then (ii); but this property is intrinsic to our formulation based on Nelson's theorem. Thus, Chow's theorem does indeed hold within our restricted treatment of the quantum control problem. To be more specific, case (b) of the theorem as stated in Sec. IIIB applies, with $\mathsf{M} \cap \mathscr{D}_\omega$, $\{H_0, H_1, ..., H_r\}$, ψ, and ψ_o playing the roles of M, $\{X_0, X_1, ..., X_r\}$, m, and m_o, respectively.

Having these basic tools at our command it is routine to generalize the remaining results for the finite-dimensional control problem (3) to the quantum case, while exercising due care with regard to domains, norms, and limits. The details of this process, available in Ref. 43, are too lengthy to reproduce here. The upshot is that so far as Theorems 3.2 and 3.3 (Sussmann and Jurdjevic) are concerned, m goes over to ψ and M to $\mathsf{M} \cap \mathscr{D}_\omega$, and, of course, X_k is replaced by H_k, $k = 0,1,...,r$, in forming the Lie algebras $\mathscr{A}$ and $\mathscr{C}$. (*N.B.*: $\mathscr{V}(\mathsf{M})$ is reinterpreted as the set of all real, analytic vector fields on $\mathsf{M} \cap \mathscr{D}_\omega$.) The important results of Kunita are also readily adapted to the quantum problem, by making the same replacements. Because of its role in the examples to be presented in Sec. V, we recast Corollary 3.5.1 explicitly in these terms.

Corollary 3.5.1': Let $\mathscr{C} = \{\mathrm{ad}^j_{H_0} H_l \,|\, l = 1,...,r;\ j = 0,1,\cdots\}_{\mathrm{LA}}$ be the ideal in $\mathscr{A} = \{H_0, H_1, ..., H_r\}_{\mathrm{LA}}$ generated by $H_1, ..., H_r$. Suppose that $\dim \mathscr{C}(\zeta) = d < \infty$, $\forall \zeta \in \mathsf{M} \cap \mathscr{D}_\omega$, and that $[\mathscr{C}, \mathscr{B}] \subset \mathscr{B}$. The quantum control system is then strongly analytically controllable on M.

The "practical" implication of this corollary is that (assuming the requisite conditions are met) we can always control the system so the state ψ, starting at any point $\psi_o \in \mathsf{M} \cap \mathscr{D}_\omega$, arrives arbitrarily close to any desired point in M after any chosen time interval t. Consequently, the expectation value of any observable quantity can be made to approach arbitrarily closely the expectation value of that quantity in any prescribed state vector in $\mathsf{M} \subset \mathscr{H}$, at any $t > 0$.

C. Controllability on $\mathsf{S}_{\mathscr{H}}$

Since Nelson's theorem requires that $\{H_0, H_1, ..., H_r\}$ gives rise to a finite-dimensional Lie algebra, it is apparently *not* possible to control the system on the unit sphere $\mathsf{S}_{\mathscr{H}}$ (i.e., with $\mathsf{M} = \mathsf{S}_{\mathscr{H}}$ in the definition of analytic controllability) if that theorem is in force. This is indeed the situation, the manifold M which enters the results of Sec. IVB being necessarily finite-dimensional. A more concise formal statement is given below.

Theorem 4.2: If $\{H_0,H_1,...,H_r\}$ generates a d-dimensional Lie algebra $\mathscr{A}$ which admits an analytic domain $\mathscr{D}_\omega$, the quantum system is not analytically controllable on $S_{\mathscr{H}}$ if d is finite.

Proof: By the properties of an analytic domain, there exists a connected, d-dimensional Lie group Γ with Lie algebra $\mathscr{A}$, the elements of Γ being constructed as $G = \exp X$ from members X of $\mathscr{A}$. Moreover, Γ can be chosen to act on $S_{\mathscr{H}} \cap \mathscr{D}_\omega$ according to $G(\xi) = (\exp X)\xi, \xi \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$. Let $\mathscr{T}$ be an e-dimensional tangent subspace of $S_{\mathscr{H}}$ at ξ, and let P: $\mathscr{H} \to \mathscr{T}$ be the corresponding orthogonal projection from $\mathscr{H}$. Then $P(G\xi)$ defines a map from the d-dimensional Lie group Γ into the e-dimensional tangent subspace $\mathscr{T}$. This map cannot be onto if $e > d$. Further, since H_0 does not enter with an adjustable control factor $u_0(t)$, the dynamical semigroup Γ_s of the quantum system (1)–(2) is contained in the group Γ. Accordingly, if (as has been shown) Γ is not sufficiently rich to steer the state trajectory into all directions of $\mathscr{T}$, neither is Γ_s, and we conclude that the system is not analytically controllable on $S_{\mathscr{H}}$.

Corollary 4.2.1: If the quantum system is analytically controllable on $S_{\mathscr{H}}$, then $\mathscr{A}$ must be infinite-dimensional.

Proof: Direct observation.

Remark: In the case that $\mathscr{A}(\xi)$ is infinite-dimensional for all $\xi \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$, an *arbitrary* flow of Γ would have the form $G(\xi) = [\Pi_j \exp s_j X^{(j)}]\xi, X^{(j)} \in \mathscr{A}, s_j \in \mathbb{R}, \{j\}$ infinite. In other words, if $\mathscr{A}(\xi)$ is infinite-dimensional, an infinite sequence of switchings would, in general, be required to build an element of Γ_s. Thus, within the context of piecewise-constant controls, practical realization of complete control of the quantum system (in the sense of analytic or strong analytic controllability on $S_{\mathscr{H}}$) is out of the question. Accordingly, our efforts have focused on the issue of controllability on finite-dimensional submanifolds of $S_{\mathscr{H}}$.

V. EXAMPLES

Example 1: In the context of a position or x representation[44] for state vectors and operators of $\mathscr{H}$, $x \in \mathbb{R}^1$, define

$$K_\pm = \pm \frac{1}{\sqrt{2}}\left(\frac{d}{dx} \mp x\right), \quad K_3 = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2}, \tag{7}$$

together with $E =$ identity operator. The operators $-iK_3$, $K_+ - K_-$, and $i(K_+ + K_-)$ are skew-Hermitian, and the Lie bracket among them is specified through[45]

$$[K_3,K_\pm] = \pm K_\pm, \quad [K_+,K_-] = -E. \tag{8}$$

Making the identifications $H_0 = -iK_3$, $H_1 = K_+ - K_-$, and $H_2 = i(K_+ + K_-)$, we consider the system

$$\frac{d}{dt}\psi(t) = \{-iK_3 + u_1(t)[K_+ - K_-] + u_2(t)[i(K_+ + K_-)]\}\psi(t), \quad \psi(0) = \psi_o. \tag{9}$$

[For notational convenience we suppress, in (9), the fact that $\psi(t) = \psi(x;t)$ depends on the variable x, and that the derivatives entering should actually be partial derivatives.] The Lie algebra $\mathscr{L}(-iK_3,K_+ - K_-, i(K_+ + K_-)) = \mathscr{A}$ has basis $-iK_3, K_+ - K_-, i(K_+ + K_-), iE$ over $\mathbb{R}^1$, and it is well known[33,45] that there is a common dense invariant domain—an analytic domain $\mathscr{D}_\omega$—for these operators, spanned by analytic functions $\phi_n(x)$. Explicitly,

$$\phi_n(x) = \pi^{-1/4}(n!)^{1/2}(-1)^n 2^{-n/2} \exp[-x^2/2] h_n(x), \quad n = 0,1,2,...,\infty, \tag{10}$$

where the $h_n(x)$ are Hermite polynomials. As basis of the Lie algebra $\mathscr{L}(K_+ - K_-, i(K_+ + K_-)) = \mathscr{B}$ one has simply $K_+ - K_-, i(K_+ + K_-), iE$. This basis is in fact shared by the ideal $\mathscr{C}$ in $\mathscr{A}$ generated by $H_1 = K_+ - K_-$ and $H_2 = i(K_+ + K_-)$. Thus the Lie algebras $\mathscr{B}$ and $\mathscr{C}$ coincide, and the property $X \in \mathscr{C}, Y \in \mathscr{C} \Rightarrow [X,Y] \in \mathscr{B}$ emerges trivially. Furthermore, we verify from (7) and (10) [or (8)] that $\dim \mathscr{A}(\omega) = \dim \mathscr{B}(\omega) = \dim \mathscr{C}(\omega) = d = 3$ for all $\omega \in \mathscr{D}_\omega$; moreover, $\dim \mathrm{I}(\mathscr{C},\xi) = 3$ for all $\xi \in S_{\mathscr{H}} \cap \mathscr{D}_\omega$. The essential relations are

$$K_+\phi_n = (n+1)^{1/2}\phi_{n+1}, \quad K_-\phi_n = n^{1/2}\phi_{n-1}, \quad K_3\phi_n = (n+\tfrac{1}{2})\phi_n, \quad E\phi_n = \phi_n. \tag{11}$$

[For the special case $\omega = \phi_o$, we have $K_-\omega = 0$. However, even in that case we obtain in effect three linearly independent vectors upon application of the basis operators $-iK_3$, $K_+ - K_-$, $i(K_+ + K_-)$, iE, since our Lie algebras are defined over the reals.]

By virtue of the properties just displayed, Corollary 3.5.1′ (stated in Sec. IVB) comes into play, and we may conclude that (i) the reachable set of ψ_o in $S_{\mathscr{H}} \cap \mathscr{D}_\omega$ is given by $\mathrm{I}(\mathscr{C},\psi_o) = \mathrm{I}(\mathscr{B},\psi_o)$ for $\psi_o \equiv \psi(0) \in \mathrm{span}\{\phi_n(x), n = 0,1,2,...,\infty\}$ and (ii) putting $\mathsf{M} = c\ell\,\mathrm{I}(\mathscr{B},\psi_o)$, the system is strongly analytically controllable on M.

At a more intuitive level, one can argue from (11) that the dynamical effect of $H_0 = K_3$ can be cancelled by that of some input which dominates $\mathscr{B}$; this implies strong analytic controllability, checking the implication of Corollary 3.5.1′.

Physically, the state-evolution equation of (9), multiplied by i, may be interpreted as the Schrödinger equation governing the dynamics of a one-dimensional quantum oscillator coupled independently via its momentum and position operators to external controls (fields) $u_1(t)$ and $u_2(t)$, respectively. The operator K_3 represents the energy of the uncoupled oscillator, while K_+ and K_- serve, respectively, as creation and destruction operators for harmonic excitations.

Example 2: The commutation relations (8) bring to mind the commutation relations for the spherical components of the angular momentum operator $\mathbf{J}$. Given the Cartesian components J_x, J_y, J_z of $\mathbf{J}$, we form the spherical components $J_\pm = J_x \pm iJ_y$, $J_3 = J_z$ and obtain[45]

$$[J_3,J_\pm] = \pm J_\pm, \quad [J_+,J_-] = 2E. \tag{12}$$

We note that (12) coincides with (8) *except* for the presence of a factor 2 on the right-hand side of the last relation, instead of a factor -1. It is evident that one can go on to formulate simple examples of the quantum controllability problem based on the Lie algebra $\mathscr{L}(-iJ_x, -iJ_y, -iJ_z)$ of the angular momentum operators.

In particular, one might set $H_0 = -iJ_z$, $H_1 = -iJ_x$, and $H_2 = -iJ_y$, and consider the system equation

$$\frac{d}{dt}\psi(t) = \{ -iJ_3 + u_1(t)[J_+ - J_-] + u_2(t)[i(J_+ + J_-)]\}\psi(t),$$
$$\psi(0) = \psi_o, \tag{13}$$

wherein we revert to our earlier interpretation of $\psi(t)$ as an element of the abstract state space. The resemblance between problems (13) and (9) is strong; for instance, we find the corresponding properties that $\mathscr{A}$ has basis $-iJ_z$, $-iJ_x$, $-iJ_y$, $-iE$, and that $\mathscr{B}$ and $\mathscr{C}$ share the basis $-iJ_x$, $-iJ_y$, $-iE$. On the other hand, an important distinction must be recognized. In the present case there exists a Casimir operator, i.e., a (non-trivial) function of base elements of the Lie algebra $\mathscr{A}$ which commutes with all base elements, whereas in Example 1 there is no such (nontrivial) operator. Here the Casimir operator is, of course, the square of the angular momentum, $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$. Thus, if we suppose that the state of the quantum system is initially in a subspace of eigenvalue $j(j+1)$ of $\mathbf{J}^2$, where $j \geqslant 0$ is integral or half-odd integral, it will always remain in that subspace. Having chosen a definite value of j, and having agreed that J_x, J_y, J_z and functions of them are the *only* relevant observables [as is the case for the particular system (13) and notably for situations in which only spin degrees of freedom are manifest], we have a problem involving a *finite-dimensional* state space χ_j, of dimension $2j+1$. Accordingly, the results of Sec. IIIB 3–4 are directly applicable, and, taking account of the skew-Hermitian nature of H_0 and the H_l, it follows that strong complete controllability prevails on the unit sphere in χ_j. Numerous explicit physical examples of this sort are encountered in the fields of atomic- and molecular-beam experiments and magnetic resonance; for archetypal cases, see Ref. 46.

Example 3: Consider the system

$$i\frac{d}{dt}\psi(t) = [P_1^2 + P_2^2 + u_1(t)P_1 + u_2(t)P_2]\psi(t),$$
$$\psi(0) = \psi_o, \tag{14}$$

where P_1 and P_2, in the x_1x_2 representation, $x_1x_2 \in \mathbb{R}^2$, have the modes of action $-i\partial/\partial x_1$ and $-i\partial/\partial x_2$, respectively. The common eigenfunctions of the commuting operators P_1, P_2 do not lie in $L^2(\mathbb{R}^2)$ and so do not qualify as representatives of Hilbert-space state vectors; however, we know from the theory of Fourier transforms that these common eigenfunctions span $L^2(\mathbb{R}^2)$ in the sense of integral superpositions. In terms of such Fourier-integral superpositions, one may in fact define a common, dense, invariant domain of $L^2(\mathbb{R}^2)$ for the unbounded operators $H_0 = -i(P_1^2 + P_2^2)$, $H_1 = -iP_1$, and $H_2 = -iP_2$. Moreover, the solution of the Schrödinger dynamical problem (14), with initial value ψ_o in the latter domain, can be expressed in exponential form. The foregoing heuristic sketch indicates that it is possible to construct a suitable analytic domain $\mathscr{D}_\omega$ for the control problem specified by (14). A rigorous construction can be formulated in terms of Nelson's theorem as stated in Sec. IV, with $T = (P_1^2 + P_2^2)^2 + P_1^2 + P_2^2$.

Now let $\psi_{k_1k_2}$ be a common eigenvector of P_1 and P_2 with respective eigenvalues k_1 and k_2, or, more properly, a wave packet or eigendifferential[44] constructed as an integral superposition of eigenvectors of these operators with respective eigenvalues lying in arbitrarily narrow intervals centered on k_1, k_2. We are faced in this example with a degenerate situation in which H_0, H_1, and H_2 all commute with one another. Thus, $[\mathscr{B},\mathscr{C}]$ collapses to the null set. Consequently, the chosen state $\psi_{k_1k_2}$ belongs to the reachable set $\mathsf{R}(\psi_o)$ only if $\psi_o = c(0)\psi_{k_1k_2}$, $|c(0)|^2 = 1$; under this condition the system always stays on the one-dimensional manifold defined by $c(t)\psi_o$, with $|c(t)|^2 = 1$. The controls $u_1(t)$ and $u_2(t)$ can at most change the phase of the state and hence are ineffectual, since all physical predictions are independent of this phase.

One may of course interpret the Schrödinger equation of (14) as that for two equal-mass particles moving in one dimension. The particles do not interact with one another, but are coupled independently via their respective momenta to controls (fields) $u_1(t)$ and $u_2(t)$.

VI. SUMMARY AND OUTLOOK

It has been our aim to lay a foundation for the concept of controllability of quantum-mechanical systems. Referring to expressions (1) and (2), a quantum control system is characterized by its internal Hamiltonian $H_0' = i\hbar H_0$, which is the infinitesimal generator of the free evolution of the quantum object, together with the operators $H_1' = i\hbar H_1, \ldots, H_r' = i\hbar H_r$, which couple that object to external controls of respective amplitudes $u_1(t), \ldots, u_r(t)$. Working within traditional quantum theory, where the H_k ($k = 0,1,\ldots,r$) are linear, skew-Hermitian operators, we have succeeded in deriving conditions for global controllability on a certain finite-dimensional submanifold of the physical Hilbert space $\mathscr{H}$. The cornerstone of the associated analysis is an analytic domain $\mathscr{D}_\omega$, which we presume to exist for the given operators. The results we have obtained are natural extensions of well-known systems-theoretic results in finite-dimensional state space (drawn especially from Refs. 10, 11, 14, 16, 17, and 19). Generalizations to nonlinear versions of the quantum control problem (corresponding to nonlinear extensions of quantum theory) have not been considered here, but some results on local controllability in the context of nonlinear operators H_k have been derived in Ref. 43. The present work on the quantum controllability problem has provided a background for investigation of the invertibility of quantum-mechanical systems[47] and the formulation of a quantum nondemolition filter.[48,49]

Still, only a modest beginning has been made toward achieving the larger goal of a comprehensive theory of quantum control and filtering. The following problems, among others, await concerted effort:

(i) Generalization of the present treatment of quantum controllability to a less restrictive scene of action than a domain of analytic vectors—for example, a domain composed of vectors of $\mathscr{H}$ for which the orbits are infinitely differentiable functions of the group parameters.

(ii) Investigation of controllability for the case of control functions $u_l(t)$ belonging to $L^2(\mathbb{R})$.

(iii) Study of a controlled version of the Schrödinger equation for the time evolution of the density operator,[44] so as to extend control theory to the realm of quantum statistical mechanics.

(iv) Adaptation of the notions of observability, identification, realization, and feedback to the quantum setting.

It is evident that powerful mathematical techniques must be invoked to carry through this program; moreover, one must confront the profound conceptual obstacles intrinsic to the quantum measurement process.[50–52]

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Convergence of the T-matrix approach in scattering theory. II

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Convergence of the T-matrix scheme is proved under more general assumptions than in Ramm [J. Math. Phys. **23**, 1123–5 (1982)] and for more general boundary conditions. Stability of the numerical scheme towards small perturbations of data and convergence of the expansion coefficients are established. Dependence of the rate of convergence on the choice of basis functions is discussed. Dependence of the quality of expansions in various spherical waves on the shape of the obstacle is discussed.

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1. INTRODUCTION

1. Let $\mathscr{D}$ be a bounded obstacle with the boundary Γ. Consider the following problem:

$$(\nabla^2 + k^2) u = 0, \quad \text{in } \Omega \quad k>0, \tag{1}$$

$$u|_\Gamma = f, \tag{2}$$

$$r\left(\frac{\partial u}{\partial r} - iku\right) \to 0, \quad r \to \infty, \tag{3}$$

where Ω is the exterior domain and f is given. Later we discuss other boundary conditions than (2), but the basic arguments and conclusions will be similar to those for problem (1)–(3).

The corresponding scattering problem is as follows: find the solution to Eq. (1) satisfying boundary condition (2) with $f = 0$ and of the form $u = u_0 + v$, where v satisfies the radiation condition (3) and u_0 is the incident field. It is clear that this problem reduces to problem (1)–(3) for v with $f = -u_0$ on Γ. Therefore, we discuss in what follows problem (1)–(3). There is an extensive literature about this problem. The existence and uniqueness of the solution to this problem for Liapunov boundaries are established long ago and are available in textbooks now.[1] The case of nonsmooth boundaries was also treated.[2] Numerical methods for solving problem (1)–(3) are known (finite differences, see e.g., Ref. 3, numerical solution of the boundary integral equations of the second and first kind[4]).

Our concern is with the T-matrix scheme.[5] This numerical scheme was widely used during the last decade in the problems of acoustic, electromagnetic, and elastic wave scattering by one and many bodies, for scattering from periodic structures etc.[5–10]

Nevertheless, the basic questions concerning convergence of the scheme, stability of the numerical scheme towards small perturbations of the data remained open. In Ref. 11 these questions were answered for the first time. Here the results from Ref. 11 are strengthened and extended.

2. Let us describe the T-matrix scheme in a general formulation. Let $\{\psi_n\}$ be a system of outgoing (not necessarily spherical) wave, i.e.

$$(\nabla^2 + k^2)\psi_n = 0 \quad \text{in } \Omega, \tag{4}$$

$$r\left(\frac{\partial \psi_n}{\partial r} - ik\psi_n\right) \to 0, \quad r \to \infty. \tag{5}$$

From the Green's formula it follows that

$$\int_\Gamma \psi_n \frac{\partial u}{\partial N_s} dS = \int_\Gamma u \frac{\partial \psi_n}{\partial N_s} dS, \quad \forall n, \tag{6}$$

where u is the solution to (1)–(3) and N is the exterior unit normal on Γ (pointing out, into Ω). Using boundary condition (2), one writes (6) as

$$\int_\Gamma \psi_n h \, dS = f_n, \quad \forall n, \tag{7}$$

where

$$f_n \equiv \int_\Gamma f \frac{\partial \psi_n}{\partial N_s} dS, \tag{8}$$

$$h \equiv \left.\frac{\partial u}{\partial N}\right|_\Gamma. \tag{9}$$

The T-matrix scheme consists of the following. Let $\{\phi_j\}$ be a linearly independent and complete system of functions in $H_0 = L^2(\Gamma)$. Let

$$h_m = \sum_{j=1}^m c_j^{(m)} \phi_j, \tag{10}$$

where $c_j^{(m)}$, $1 \leqslant j \leqslant m$, are constant coefficients, which should be defined from the linear algebraic system

$$\sum_{j=1}^m a_{nj} c_j^{(m)} = f_n, \quad 1 \leqslant n \leqslant m, \tag{11}$$

$$a_{nj} = \int_\Gamma \psi_n \phi_j \, dS \equiv (\phi_j, \bar{\psi}_n). \tag{12}$$

One obtains this system if (10) is substituted in (7) and only the first m equalities (7) are used.

3. Justification of the T-matrix scheme requires positive answers to the following questions:

Q1. Is (11) solvable for sufficiently large m?

Q2. Does $h_m \xrightarrow[H_0]{} h$, $m \to \infty$? Here h is defined as in (9).

Q3. Does $c_j^{(m)} \to c_j$, $m \to \infty$? Is the convergence uniform in j, $1 \leqslant j < \infty$?

Q4. Does the equality $h = \sum_{j=1}^\infty c_j \phi_j$ hold, where c_j are defined in Q3, and it is assumed the limits c_j exist?

Q5. How does the rate of convergence depend on the

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choice of the systems $\{\phi_j\}$ and $\{\psi_n\}$?

Q6. Is the numerical scheme based on Eq. (11) stable towards small perturbations of f_n and the matrix a_{nj}?

Remark 1: In the literature[12] the following questions were discussed: Is the set of Eqs. (7) solvable? Is the solution to (7) unique? These questions are easy to answer. The set of Eqs. (7) is solvable for any system $\{\psi_n\}$ satisfying (4) and (5): Take the solution u to (1)–(3) (which does exist) and apply Green's formula to ψ_n and u to obtain (7). The solution to (7) is unique iff the system $\{\psi_n\}$ is closed in $H_0 \equiv L^2(\Gamma)$ so that

$$\int_\Gamma h\,\psi_n\,dS = 0,\ \forall n \quad \Rightarrow \quad h = 0. \tag{13}$$

This is equivalent to saying that any $h \in H_0$ can be approximated with prescribed accuracy ϵ in the norm of H_0 by linear combinations of the elements ψ_n: $\| h - \Sigma_{j=1}^{m(\epsilon)} c_j(\epsilon)\,\psi_j \| < \epsilon$, i.e., the system $\{\psi_j\}$ is complete. We assume below that the system $\{\psi_j\}$ is closed.

4. If one takes as ψ_1 in (7) $g(s,y) = g(s,y,k) = \exp(ik\,|s-y|)/4\pi|s-y|, y \in \mathscr{D}$, and does not use Eqs. (7) for $n > 1$, then one gets the integral equation

$$\int_\Gamma g(s,y)\,h(s)\,dS = \int_\Gamma f(s)\,\frac{\partial g(s,y)}{\partial N_s}\,dS \equiv F(y), \quad y \in \mathscr{D}. \tag{14}$$

Actually, if (14) holds for $y \in B \subset \mathscr{D}$, where B is any ball lying strictly in $\mathscr{D}$, then (13) holds in $\mathscr{D}$ because both sides in (14) are solutions to the Helmholtz equation in $\mathscr{D}$, and, therefore, if they are identical in B, they are identical in $\mathscr{D}$. If one lets $y \to s' \in \Gamma$, one obtains from (14) the boundary integral equation of the first kind

$$Ah = \int_\Gamma g(s,s')\,h(s)\,dS = b(s'), \tag{15}$$

where

$$b(s') \equiv \lim F(y), \quad y \in \mathscr{D},\ y \to s'. \tag{16}$$

If one looks for a solution of (15) of the form (10) and uses a projection method for finding $c_j^{(m)}$, one obtains the system

$$\sum_{j=1}^{m} A_{nj}\,c_j^{(m)} = b_n, \quad 1 \leqslant n \leqslant m, \tag{17}$$

where

$$A_{nj} \equiv (A\phi_j, \eta_n), \quad b_n \equiv (b, \eta_n), \tag{18}$$

$$(f,h) \equiv \int_\Gamma f\bar{h}\,dS, \tag{19}$$

and the bar denotes complex conjugation. The same questions Q1–Q6 can be studied for system (17). In this case η_n plays the role of ψ_n, but now there is no need to assume anything about the properties of η_n in Ω. In fact, η_n are defined only on the surface Γ. Questions Q1, Q2, Q5, and Q6 were answered in Ref. 11 for the system (17) under the assumption that $\eta_n = \phi_n$ and the system $\{\phi_n\}$ forms a basis of $H_{-1/2}$. The spaces $H_q = W_2^q(\Gamma)$, $-\infty < q < \infty$, are defined as the spaces of functions with q square integrable derivatives for $q \geqslant 0$ integer, and as dual spaces (spaces with negative norm) for $q < 0$. For arbitrary $q < 0$ they can be defined as interpolating spaces, or directly.[13] In the present paper we note that the result and arguments in Ref. 11 are valid under the weaker assumption that $\{\phi_j\}$ is a complete system of linearly independent functions (not necessarily a basis; see Sec. 2.3 below).

From the integral equation (14) one can go back to the system (7) assuming that

$$g(s,y) = \sum_{j=1}^{\infty} \phi_j(y)\,\psi_j(s), \quad |y| < |s|, \tag{20}$$

substituting (20) into (14), and equating coefficients in front of ϕ_j. From this point of view the integral equation (14) is equivalent to the system (7)–(8). In the literature, expansion (20) is used, with ψ_j being the outgoing spherical waves and ϕ_j being the regular (i.e., finite at the origin) solutions to Helmholtz' equation. Matrix (18) will be identical to matrix (12) if ψ_n in (12) are chosen so that $A\bar{\eta}_n = \psi_n$. This corresponds to a specific choice of the outgoing waves, since for any linearly independent system of functions η_n in $L^2(\Gamma)$, the system $\psi_n \equiv A\bar{\eta}_n$ will be a system of outgoing waves whose boundary values on Γ form a linearly independent system in $L^2(\Gamma)$, provided that the operator $A: L^2(\Gamma) \to L^2(\Gamma)$ has no zeros (i.e., $A\eta = 0 \Rightarrow \eta = 0$). This will be the case iff k^2 is not an eigenvalue of the interior Dirichlet Laplacian in $\mathscr{D}$.

In Ref. 11 it was noted that, in the case when k^2 is an eigenvalue of the Dirichlet Laplacian in $\mathscr{D}$, one can use, instead of $g(x,y,k)$, the Green's function $g_\epsilon(x,y,k)$ and in this case the corresponding operator A will have no zeros. The function g_ϵ is the Green's function of the Dirichlet operator $\nabla^2 + k^2$ in the exterior of a small ball B_ϵ situated in $\mathscr{D}$, where B_ϵ is so chosen that k^2 is not an eigenvalue of the problem

$$(\nabla^2 + k^2)\,u = 0 \quad \text{in } \mathscr{D} \setminus B_\epsilon, \quad u|_\Gamma = 0, \quad u|_{\partial B_\epsilon} = 0,$$

where ∂B_ϵ is the boundary of B_ϵ, and $\mathscr{D} \setminus B_\epsilon$ is the complement in $\mathscr{D}$ to B_ϵ.

The above argument shows that the analysis in Ref. 11 is applicable to Eq. (11) under some special choice of ψ_n in (12).

In Refs. 13–23 some results in functional analysis, theoretical numerical analysis, scattering theory, and special functions are given. These results will be specified and used in Secs. 2–4 and in the appendices.

2. ANALYSIS OF THE T-MATRIX SCHEME

In this section we discuss questions Q1–Q6 formulated in Sec. 1.3.

1. The system (11) is solvable for a given m iff $\det(a_{nj})_{n,j=1}^m \neq 0$. For the following analysis we need some definitions and results from the theory of Hilbert spaces. These definitions and results are given in Appendix A. In Appendix C some results about convergence and stability of projection methods are given.

We are interested in the properties of the coordinate systems $\{\phi_j\}$ and $\{\psi_j\}$, which imply positive answers to questions Q1, Q2, Q3, and Q6. Let us write Eq. (7) as an operator equation

$$ah = \hat{f}, \quad a\colon H_0 \to l^2, \quad H_0 = L^2(\Gamma), \quad \hat{f}(f_1, f_2, \ldots), \tag{7'}$$

where the operator a is bounded and defined on all of H_0 iff

$$\sum_{n=1}^{\infty} |(h,\bar{\psi}_n)|^2 \leqslant c_2^2 \int_\Gamma |h|^2 dS,$$

$$\forall h \in H_0, \ c_2 > 0.$$

If this inequality does not hold for all $h \in H_0$, but the system $\{\psi_n\}$ is a basis of H_0, then a is densely defined [i.e., its domain $D(a)$ is dense in H_0]. Indeed, in this case the biorthogonal system $\{\tilde{\psi}_n\}$ is also a basis of H_0 (Ref. 17, p. 307), and any linear combination $\Sigma_{j=1}^m c_j \tilde{\psi}_j \in D(a)$.

The operator a transforms a function $h \in H_0$ into a sequence $(h, \bar{\psi}_n) = \int_\Gamma h\psi_n \, dS$, $1 \leqslant n < \infty$. The range of a is dense in l^2 provided that for any sequence $\{d_n\} \in l^2$ the series $\Sigma_{n=1}^\infty d_n \psi_n(x)$ converges in H_0 and the system $\{\psi_n\}$ is ω-linearly independent, i.e., $\Sigma_{n=1}^\infty d_n \psi_n = 0 \Leftrightarrow d_n = 0$, $\forall n$. Indeed, suppose that $(ah, d) = 0$, $\forall h \in H_0$, where the parentheses denote the inner product in l^2. Then $\int_\Gamma h \, \Sigma_{n=1}^\infty \bar{d}_n \psi_n \, dS = 0$. Since $h \in H_0$ can be taken arbitrary, it follows that $\Sigma_{n=1}^\infty \bar{d}_n \psi_n = 0$ and $d_n = 0$, $\forall n$. The operator a^{-1} will be bounded and defined on all of l^2 iff $\| ah \| \geqslant c_1 \| h \|$, $\forall h \in H_0, c_1 > 0$. We use the same notation for the norms in H_0 and l^2. This inequality can be written as

$$\sum_{n=1}^{\infty} |(h,\bar{\psi}_n)|^2 \geqslant c_1^2 \int_\Gamma |h|^2 dS, \quad \forall h \in H_0, \ c_1 > 0.$$

Therefore, a and a^{-1} are both bounded iff

$$c_1^2 \| h \|^2 \leqslant \sum_{n=1}^{\infty} |(h,\bar{\psi}_n)|^2 \leqslant c_2^2 \| h \|^2, \quad \forall h \in H_0, \ c_1 > 0.$$

These inequalities hold iff the system $\{\psi_j\}$ forms a Riesz basis of H_0. Let us consider the truncated equations (7), i.e., the system (11) as a projection method for solving (7'). Namely, let Q_m be an orthoprojection in l^2 defined by the formula $Q_m \hat{f} = f^{(m)} = (f_1,...,f_m,0,0,\cdots)$, and P_m be an orthoprojection in H_0 on the linear span of $(\phi_1,...,\phi_m)$. The system (11) can be written as

$$Q_m a P_m h_m = Q_m \hat{f}, \quad P_m h_m = h_m = \sum_{j=1}^m c_j^{(m)} \phi_j. \quad (11')$$

This equation is of the type studied in Appendix C [see (C2)]. Conditions (C4) and (C5) are necessary and sufficient for Eq. (11') [i.e., (11)] to be uniquely solvable for all sufficiently large $m > m_0$ and for the convergence

$$\| h_m - h \| \to 0, \quad m \to \infty. \quad (21)$$

Conditions (C4) can be written in our case as

$$\sum_{n=1}^m \left| \sum_{j=1}^m a_{nj} c_j \right|^2 \geqslant c \int_\Gamma \left| \sum_{j=1}^m c_j \phi_j \right|^2 dS, \quad \forall m > m_0, \ c > 0, \quad (22)$$

where $c_1 \cdots c_m$ are arbitrary constants, $a_{nj} = (\phi_j, \bar{\psi}_n)$. Condition (22) can be written as

$$c_j \bar{c}_{j'} \, a_{nj} \bar{a}_{nj'} \geqslant c c_j \bar{c}_{j'} (\phi_j, \phi_{j'}),$$

where one should sum over repeated indices and the bar denotes complex conjugation. This last inequality means that the following matrix inequality holds:

$$(a^* a)_m \geqslant c(\Phi)_m, \quad \forall m > m_0, \ c > 0. \quad (22a)$$

Here $(a)_m$ is the truncated matrix: $(a)_m = (a_{nj})_{n,j=1}^m$. $\Phi = (\phi_j, \phi_{j'}) = \int_\Gamma \phi_j \bar{\phi}_{j'} \, dS$ is the Gram matrix for the system $\{\phi_j\}$. If $\lambda(\Phi)$ [$\Lambda(\Phi)$] denotes the minimal [maximal] eigenvalue of a self-adjoint matrix $\Phi \geqslant 0$, then (22a) holds if, for example

$$\inf_m \lambda((a^* a)_m) \geqslant \lambda > 0, \quad \sup_m \Lambda((\Phi)_m) \leqslant \Lambda < \infty. \quad (22b)$$

This condition is convenient from a practical point of view. The conclusion is as follows: if (22b) holds, then the projection method (11) for solving Eqs. (7) converges, i.e., Eqs. (11) are uniquely solvable for sufficiently large $m > m_0$ and $\| h_m - h \| \to 0$ as $m \to \infty$, where h is the solution of (7). The second equality (22b) holds, for example, if the system $\{\phi_j\}$ forms a Riesz basis of H_0. If we take $\phi_j = \bar{\psi}_j$ on Γ, then $a = \Phi$ and inequality (22a) holds iff the first inequality (22b) holds. Indeed, if $a = \Phi$, then (22a) takes the form $(a^2)_m \geqslant c(a)_m$, $m > m_0$, $a = a^*$. This inequality holds iff the spectrum of $(a)_m$ is bounded away from zero by a positive constant. To see this, let us use the spectral theorem for the self-adjoint operator $a \geqslant 0$:

$$((a^2 - ca)\phi, \phi) = \int_0^\infty (t^2 - ct) \, d(E_t \phi, \phi),$$

where E_t is the resolution of the identity for a, $\min_{t>0} (t^2 - ct) = -c^2/4$, $t^2 - ct \geqslant 0$ if $t \geqslant c$. Therefore, the operator $a^2 - ca$ will be nonnegative for some $c > 0$ iff $a \geqslant \alpha > 0$, where α is a positive constant and in this case we can take $\alpha = c$ in the inequality (22a). Note that $\alpha = \lambda^{1/2}$, where λ is the constant in (22b). If the system $\{\phi_j\}$ is such that $\inf_m \lambda((\Phi)_m) \geqslant \lambda > 0$ (in particular, if it is a Riesz basis of H_0), then the conclusion is as above [after formula (22b)].

Condition (C5) means that for $m > m_0$ the set of vectors $\{a_{nj}\}_{n=1}^m$, $1 \leqslant j \leqslant m$, is linearly independent. That is,

$$\det(a_{nj})_{j,n=1}^m \neq 0, \quad \forall m > m_0. \quad (23)$$

This condition follows from (22) [see Remark 1 in Appendix C and formula (22b)].

If (22) holds, then system (11) is uniquely solvable for all $m > m_0$, and the function (10), where $\{c_j^{(m)}\}$, $1 \leqslant j \leqslant m$, is the solution of (11), converges in H_0 to the solution of (7). The rate of the convergence is given by (C8). This rate depends on the rate of convergence of $(I - P_m) h$ to zero, i.e., on the rate of approximation of the function $h = a^{-1} f$ by the linear combinations $\Sigma_{j=1}^m c_j \phi_j$. Stability of the solution towards small perturbations of the operator (i.e., of the matrix a_{nj}) and the right-hand side f (i.e., the sequence $\{f_n\}$) follow from the result (1) in subsection 2 of Appendix C. Indeed, consider the perturbed system

$$\sum_{j=1}^m (a_{nj} + b_{nj}) \tilde{c}_j^{(m)} = f_n + \epsilon_n, \quad 1 \leqslant n \leqslant m, \quad (11'')$$

where b_{nj} and ϵ_n are the small perturbations of the operator a and the right-hand side f, respectively. Let b_{nj} be sufficiently small in the sense that the operator b corresponding to the matrix b_{nj} is sufficiently small in the norm: $\| b \| < \delta$. Here b: $H_0 \to l^2$ can be considered as an operator which is defined as follows. The system $\{\psi_n\}$ is perturbed: $\tilde{\psi}_n = \psi_n + \eta_n$. This perturbation generates the perturbation b of a by the formula $bh = (h, \bar{\eta}_n)$. The matrix b_{nj} is then defined as $(\phi_j, \bar{\eta}_n)$. If $\| b \| < \delta$ and $\delta < c$, where c is the constant in (22) [or C4)], then according to the result (1) in subsection 2 of Appendix C, the perturbed system (11″) will be uniquely solvable for all sufficiently large m and the corresponding $\tilde{h}_m = \Sigma_{j=1}^m \tilde{c}_j^{(m)} \phi_j$ will tend to $\tilde{h} = \tilde{a}^{-1}\tilde{f} = (a+b)^{-1}(f+f_\epsilon)$, where $f_\epsilon = (\epsilon_1, \epsilon_2, \cdots)$, $\|f_\epsilon\| < \epsilon$. Thus

$$\| \tilde{h} - h \| = \|(a+b)^{-1}f - a^{-1}f + (a+b)^{-1}f_\epsilon\| \leqslant c'(\epsilon + \delta). \tag{24}$$

The constant c' can be specified:

$$c' = \|(a+b)^{-1}\| + \|f\| \, \|a^{-1}\| \, \|(a+b)^{-1}\|. \tag{25}$$

Here we used the identity $(a+b)^{-1} - a^{-1} = -(a+b)^{-1}ba^{-1}$ and the estimate $\|(a+b)^{-1} - a^{-1}\| \leqslant \|(a+b)^{-1}\| \cdot \|a^{-1}\| \cdot \|b\|$, which follows from the identity.

The estimates (21), (24), and (25) and the above arguments give answers to Q1, Q2, Q5, and Q6. We now pass over to a discussion of questions Q3 and Q4.

Let us assume that

$$\{\phi_j\} \text{ is a complete minimal system in } H_0. \tag{26}$$

(For the definition of minimal systems and their properties used below, see Appendix A.) Then there exists a unique biorthogonal system $\{\tilde{\phi}_j\}, (\phi_i, \tilde{\phi}_j) = \delta_{ij}$. Equation (11) can be written as $(a)_m \, c^{(m)} = f^{(m)}$. Its solution gives $h_m = \Sigma_{j=1}^m c_j^{(m)} \phi_j$. Therefore,

$$c_j^{(m)} = (h_m, \tilde{\phi}_j). \tag{27}$$

Since $\| h_m - h \| \to 0$, we conclude that

$$c_j^{(m)} \to c_j, \quad m \to \infty. \tag{28}$$

Thus (26) implies a positive answer to Q3. We have

$$| c_j^{(m)} - c_j | \leqslant \| h_m - h \| \; \| \tilde{\phi}_j \| \leqslant \| h_m - h \| \sup_j \| \tilde{\phi}_j \|. \tag{29}$$

Therefore, the condition

$$\sup_j \| \tilde{\phi}_j \| \leqslant C < \infty \tag{30}$$

implies that convergence in (28) is uniform in j, $1 \leqslant j < \infty$. Condition (30) holds, e.g., if

$$\text{the system } \{\phi_j\} \text{ forms a Riesz basis of } H_0 \tag{31}$$

(see Appendix A). Condition (31) implies also the positive answer to Q4. Indeed, if (31) holds then h can be written as

$$h = \sum_{n=1}^{\infty} \tilde{c}_j \, \phi_j, \tag{32}$$

and the coefficients $\tilde{c}_j$ are uniquely determined by the element h. On the other hand, we know that

$$\| h_m - h \| \to 0, \quad m \to \infty, \tag{33}$$

where

$$h_m = \sum_{j=1}^{m} c_j^{(m)} \phi_j, \quad c_j^{(m)} \to c_j. \tag{34}$$

First, we conclude that $\tilde{c}_j = c_j$ because

$$\tilde{c}_j = (h, \tilde{\phi}_j) = \lim (h_m, \tilde{\phi}_j) = \lim c_j^{(m)} = c_j. \tag{35}$$

Secondly, we see from (32) and (35) that the answer to Q4 is yes.

In the above analysis the basic assumptions were (22), (26), and (31), and we explained which of these imply positive answers to which of the basic questions Q1–Q6.

2. In this section we discuss the assumptions (26) and (31) and a particular case of the matrix a_{nj} for which the convergence analysis is straightforward. Note that (26) and (31) deal only with one of the systems. Assumption (22) deals with the "interaction" between the systems $\{\phi_j\}$ and $\{\psi_j\}$.

Assumption (26) holds if the smallest eigenvalue of the matrix $\phi_{ij} \equiv (\phi_i, \phi_j)$, $1 \leqslant i, j \leqslant m$ is bounded away from 0: $\lambda_m \geqslant \lambda > 0$ (see Appendix A). Assumption (31) holds iff the matrix ϕ_{ij} defines a bounded and boundedly invertible operator on l^2 (see Appendix A). Since this is a self-adjoint matrix, this will be the case iff

$$\Lambda_m \leqslant \Lambda < \infty, \quad \lambda_m \geqslant \lambda > 0, \tag{36}$$

where Λ_m (λ_m) is the maximal (minimal) eigenvalue of the matrix ϕ_{ij}, $1 \leqslant i, j \leqslant m$.

One can measure the "interaction" between $\{\phi_j\}$ and $\{\psi_j\}$ by the operator generated by the matrix $a_{nj} - \delta_{nj} = q_{nj}$. The assumptions

$$a_{nj} = \delta_{nj} + q_{nj}, \quad \delta_{nj} = \begin{cases} 0, & n \neq j, \\ 1, & n = j, \end{cases} \quad q = (q_{nj}), \quad 1 \leqslant n, j < \infty, \tag{37a}$$

is a compact operator on l^2,

$$(I + q)x = 0, \quad x \in l^2 \Rightarrow x = 0 \tag{37b}$$

are sufficient for the unique solvability of (11) for all sufficiently large $m > m_0$, and for the convergence in l^2: $\| c^{(m)} - c \| \to 0$, $m \to \infty$, where $c^{(m)} = (c_1^{(m)} \cdots c_m^{(m)}, 0, 0 \cdots)$, $c = \tilde{a}^{-1} f$, $\tilde{a}$ is the operator on l^2 with the matrix a_{nj}. Indeed, assumptions (37a), (37b) and Fredholm's alternative imply that $\tilde{a}^{-1}$ exists, is defined on all of l^2, and is bounded. This fact and the special structure of $\tilde{a}$ imply the above statement about convergence. To see this, let us write (11) as $c^{(m)} + Q_m q c^{(m)} = f^{(m)}$, where Q_m is the orthoprojection in l^2 onto the m-dimensional space of vectors with components $c_j = 0$ for $j > m$. Since q is compact and $Q_m \to I$ strongly in l^2, one concludes that $\| q - Q_m q \| \to 0$, $m \to \infty$. Therefore, $\|(I + Q_m q)^{-1} - (I + q)^{-1}\| \to 0$, $m \to \infty$. This proves the statement about convergence of $c^{(m)}$ to c.

If the system $\{\phi_j\}$ forms a basis of $H_0 = L^2(\Gamma)$ and $f \in l^2$, then the solution of (7) is $h = \Sigma_{j=1}^\infty c_j \phi_j$, where c is the limit in l^2 when $m \to \infty$ of the solutions $c^{(m)}$ to (11) and the solution to the equation $\tilde{a}c = f$. In this case (37a) $\Rightarrow$ (37b) due to Fredholm's alternative and the uniqueness of the solution to the equation $\tilde{a}c = 0$. Let us show that $\tilde{a}c = 0 \Rightarrow c = 0$. If the system $\{\phi_j\}$ forms a basis of H_0, then Eqs. (7) and $\tilde{a}c = f$ are equivalent. But the homogeneous equations (7) have only the trivial solution if the system $\{\psi_n\}$ is closed in $H_0 = L^2(\Gamma)$. (This assumption about $\{\psi_n\}$ is very natural and was made in the very beginning, see Remark 1 in the Introduction.) Therefore, $\tilde{a}c = 0 \Rightarrow c = 0$. As our analysis shows, the behavior of the smallest and largest eigenvalue of the matrices

(ϕ_i, ϕ_j), $(\phi_i, \bar{\psi}_j)$ are of basic importance in an analysis of convergence and stability of the T-matrix scheme. For the operators of the form $a = I + q$, where q is compact, the projection scheme is discussed below in subsection 4. In this case the justification of the projection scheme can be easily obtained. In Ref. 11 the problem was reduced to a projection scheme for the equation of the above form $(I + T)h = f$, where T was compact.

3. Let us discuss briefly the results in Ref. 11 from our general point of view. The matrix analogous to A_{nj} in (18) in Ref. 11 was of the form $A_{nj} = (A\phi_n, \phi_j)$, where the operator A was defined in (15). It was noted in Ref. 11 that $A = A_0(I + T(k))$, where $A_0 > 0$ in $H_0 = L^2(\Gamma)$ and $T(k)$ is compact in H_q for any $-\infty < q < \infty$. Furthermore, A_0: $H_q \to H_{q+1}$ is a continuous linear bijection of H_q onto H_{q+1}. Therefore, $A_{nj} = [(I + T(k))\phi_n, \phi_j]$, where $[u,v] \equiv (A_0 u, v) = (u, v)_{-1/2}$ and $(u, v)_q$ being the inner product in H_q. The operator $I + T(k)$ was assumed to be invertible. This can be done without loss of generality (see Ref. 11 and our argument in the end of Sec. 1.4 above). If $\{\phi_j\}$ forms a complete set of linearly independent functions in $H_{-1/2}$, our general argument shows that the system (17) is uniquely solvable for sufficiently large m, and the answers to the remaining questions Q2–Q6 are similar to the ones given above (see Sec. 2.4 below).

In particular, we have stability as $m \to \infty$ of the numerical scheme corresponding to system (17), with the matrix $(A\phi_j, \phi_n)$ and the operator A defined in (15), with respect to small perturbations of the matrix A_{nj} and $\{b_n\}$. In Ref. 11 it was assumed that the system $\{\phi_j\}$ forms a basis of $H_{-1/2}$. This assumption is weakened here: Only completeness in $H_{-1/2}$ of the system $\{\phi_j\}$ is required. If a linearly independent system $\{\phi_j\}$ is complete in $H_0 = L^2(\Gamma)$, it will be complete in $H_{-1/2}$. Indeed, H_0 is dense in $H_{-1/2}$. Therefore, for any $f \in H_{-1/2}$ one can find $f_\epsilon \in H_0$ such that $\|f - f_\epsilon\|_{-1/2} < \epsilon$. If the system $\{\phi_j\}$ is complete in H_0, then one can approximate f_ϵ in H_0 by a linear combination: $\|f_\epsilon - \sum_{j=1}^{m(\epsilon)} c_j(\epsilon)\phi_j\|_0 < \epsilon$. Since $\|u\|_0 \geqslant \|u\|_{-1/2}$, one concludes that $\|f - \sum_{j=1}^{m(\epsilon)} c_j(\epsilon)\phi_j\|_{-1/2} < \epsilon$. This means that the system $\{\phi_j\}$ is dense in $H_{-1/2}$. (The same argument shows that this system will be dense in H_q for any $q \leqslant 0$.) This remark simplifies the argument in Ref. 11 in the case when we do not require that the system $\{\phi_j\}$ be a basis. In Ref. 11 a basis in $L^2(\Gamma)$ was constructed from the "distorted spherical harmonics" under the additional assumption that Γ is star-shaped (i.e., there exists a point in $\mathscr{D}$ from which every point of Γ can be seen).

4. Let us outline a proof of convergence of the projection method for solving the equation $u + Tu = f$ in a Hilbert space H under the assumptions that T is compact and $(I + T)^{-1}$ is bounded. The projection scheme is as follows: The approximate solution u_m is sought in the form $u_m = \sum_{j=1}^{m} c_j^{(m)}\phi_j$, where $\{\phi_j\}$ is a complete set of linearly independent elements in H. Let P_n denote the orthoprojection onto the linear span of $\{\phi_1,...,\phi_n\}$. The coefficients $c_j^{(m)}$ are to be found from the equations $(u_m + Tu_m - f, \phi_j) = 0$, $1 \leqslant j \leqslant m$. These equations can be written as an operator equation $P_m u_m + P_m T u_m - P_m f = 0$. But $P_m u_m = u_m$, and therefore $(I + P_m T)u_m = P_m f$, or $(I + T - r_m)u_m = P_m f$, where $r_m = (I - P_m)T$. Since the system $\{\phi_j\}$ is complete, $\|P_m f - f\| \to 0$ as $m \to \infty$ for any fixed $f \in H$. Therefore, $I - P_m \to 0$ strongly. This and the compactness of T imply that $\|r_m\| \to 0$. Therefore, the operator $I + T - r_m$ is boundedly invertible for sufficiently large m:

$$
\begin{aligned}
(I + T - r_m)^{-1} &= \{(I + T)[I - (I + T)^{-1}r_m]\}^{-1} \\
&= (1 - Vr_m)^{-1}V = \sum_{j=0}^{\infty}(Vr_m)^j V \quad \text{if } \|Vr_m\| < 1.
\end{aligned}
$$

Here $V = (I + T)^{-1}$. One can estimate the rate of convergence of $u_m = (I + P_m T)^{-1}P_m f$ to $u = (I + T)^{-1}f$. Indeed

$$
\begin{aligned}
\|u_m - u\| &\leqslant \|(I + P_m T)^{-1}(P_m f - f)\| \\
&\quad + \|[(I + P_m T)^{-1} - (I + T)^{-1}]f\| \\
&\leqslant \|(I + P_m T)^{-1}\|\,\|P_m f - f\| \\
&\quad + \|(I - Vr_m)^{-1}V - V\|\,\|f\|.
\end{aligned}
$$

Let $\|V\| \leqslant a$, $\|r_m\| \leqslant \epsilon_m$, and $a\epsilon_m < 1$, then

$$\|(I + P_m T)^{-1}\| \leqslant \sum_{j=0}^{\infty}(a\epsilon_m)^j a = \frac{a}{1 - a\epsilon_m},$$

$$\|(I - Vr_m)^{-1}V - V\| \leqslant \frac{a^2\epsilon_m}{1 - a\epsilon_m}.$$

These estimates show that the rate of convergence of u_m to u is determined by ϵ_m, a, and $\|P_m f - f\|$. The above argument is a particular case of a known general theory.[14]

5. So far we have discussed the case of the Dirichlet boundary condition (2). If one has the Neuman boundary condition

$$\frac{\partial u}{\partial N} = f \quad \text{on } \Gamma, \tag{2'}$$

then our arguments are essentially the same: Eqs. (6) lead to Eqs. (7) with $h = u|_\Gamma$, $f_n = \int_\Gamma \psi_n f\,dS$, and now the role of ψ_n in Eq. (7) is played by the functions $\partial\psi_n/\partial N_s$.

However, the integral equation corresponding to this case will differ from (15). Indeed, in this case from (2') and the formula

$$\int_\Gamma g(s, y)\frac{\partial u}{\partial N_s}\,dS = \int_\Gamma u\,\frac{\partial g(s, y)}{\partial N_s}\,dS, \quad y \in \mathscr{D},$$

one obtains

$$\int_\Gamma \tilde{h}\,\frac{\partial g(s, y)}{\partial N_s}\,dS = \int_\Gamma g(s, y) f\,dS \equiv F(y), \quad y \in \mathscr{D}, \tag{14'}$$

where $\tilde{h} = u|_\Gamma$.

Let $y \to s' \in \Gamma$ in the above equation. Then, using the known formula for the limit value on Γ of the potential of double layer, one obtains

$$\tilde{h} = B\tilde{h} - 2\tilde{b}, \tag{15'}$$

where

$$B\tilde{h} \equiv 2\int_\Gamma \tilde{h}(s)\frac{\partial g(s, s')}{\partial N_s}\,dS, \quad \tilde{b}(s') = \lim_{y \to s'} \tilde{F}(y). \tag{16'}$$

If one has the impedance boundary condition

$$-\frac{\partial u}{\partial N_s}+\gamma u=f \quad \text{on } \Gamma, \tag{2''}$$

then again from (6), one obtains (7) with $h=u|_\Gamma, f_n = \int_\Gamma f\psi_n \, dS$ and now the functions $-\partial\psi_n/\partial N+\gamma\psi_n$ play the role of ψ_n in Eq. (7). Completeness of all these systems in $H_0 = L^2(\Gamma)$ for the case when ψ_n are outgoing spherical waves, or any system for which the expansion

$$g(x,y)=\sum_{j=1}^{\infty}\phi_j(x)\,\psi_j(y), \quad |x|<|y|, \tag{38}$$

holds, is easily seen. For example, if

$$\int_\Gamma f\psi_n \, dS=0, \quad \forall n, \tag{39}$$

then (38) and (39) imply

$$\int_\Gamma g(x,s) f\, dS=0, \quad x\in\mathscr{D}. \tag{40}$$

Therefore $u(x)\equiv\int_\Gamma g(x,s)f\,dS$ solves the equation $(\nabla^2+k^2)u=0$ in $\mathscr{D}$ and in Ω, and $u|_\Gamma=0$. This implies that $u=0$ in Ω. If $u=0$ in Ω and in $\mathscr{D}$, then $f=(\partial u/\partial N_s)_+ -(\partial u/\partial N_s)_- =0$. Here $+$ $(-)$ denote the limit values on Γ from the interior (exterior).

3. NUMERICAL EXPERIMENTS

The purpose of the numerical computations presented here is to test whether some commonly used complete set of functions, e.g., outgoing and regular spherical waves, also satisfies the assumptions made in the previous sections. Do they, for instance, form a Riesz basis? Are they good for expansion of functions on Γ?

1. Before answering these questions, it might be illustrative to consider a simpler one-dimensional case, e.g.,

$$\phi_m(x)=\sqrt{2/\pi}\,e^{-qmx}\sin mx, \quad m=1,2,3,\cdots, \quad x\in[0,\pi]. \tag{41}$$

This set of functions is a perturbation of the orthonormal basis $\sqrt{2/\pi}\sin mx$ by factors e^{-qmx}. Here the constant q can be taken as a measure of the eccentricity of the object. The motivation for our choice of the model example will become clear from the considerations given after formulas (45). The Gram matrix of this model problem can be calculated analytically. We have

$$\begin{aligned}(\phi_m,\phi_n)&=\pi^{-1}q(m+n)\,[1-(-1)^{m+n}e^{-q\pi(n+m)}]\\ &\quad\times\{[q^2(m+n)^2+(m-n)^2]^{-1}\\ &\quad-[q^2(m+n)^2+(m+n)^2]^{-1}\}.\end{aligned} \tag{42}$$

We define the condition number for an operator A as $\kappa=\|A\|\cdot\|A^{-1}\|$.

Notice that the Gram matrix is always self-adjoint nonnegative and the finite Gram matrix is positive definite, provided the functions $\{\phi_j\}$ are linearly independent. For a positive self-adjoint operator the norms $\|A\|$ and $\|A^{-1}\|$ can be calculated by the formulas $\|A\|=\Lambda$, $\|A^{-1}\|=\lambda^{-1}$, where $\lambda=\min_{t\in\sigma(A)}t$, $\Lambda=\max_{t\in\sigma(A)}t$, and $\sigma(A)$ is the spectrum of A. In this case

$$\kappa=\Lambda\lambda^{-1}. \tag{43}$$

Numerical data seems to show that even after normalization, the perturbed system $\phi_m\sqrt{2/\pi}\,e^{-qmx}\sin mx$, $m=1,2,3,\cdots$, does not form a Riesz basis of $L^2([0,\pi])$. The nonnormalized system $\{\phi_j\}$ is not a Riesz basis because the necessary condition $0<c\leqslant\inf_{m\geqslant1}\|\phi_m\|$ for a system $\{\phi_m\}$ to form a Riesz basis is violated.

In Table I we give the condition number κ defined in Eq. (43) for both $\{\phi_m\}$ and the normalized functions $\{\phi_m/\|\phi_m\|\}$. Three different tendencies are noticed:

(1) An increase in condition number κ as the truncation size grows.

(2) An increase in condition number κ as the eccentricity grows.

(3) The normalized functions have smaller condition number as compared to nonnormalized ones

2. We now consider the spherical waves, i.e.,

$$\left.\begin{aligned}\psi_n(x)&=h_l^{(1)}(kr)\,Y_n(\omega)\\ \operatorname{Re}\psi_n(x)&=j_l(kr)\,Y_n(\omega)\end{aligned}\right\}, \quad r=|x|. \tag{44}$$

Here $h_l^{(1)}(kr)$ is a spherical Hankel function of the first kind and $j_l(kr)$ is a spherical Bessel function. The spherical harmonics $Y_n(\omega)$, where $\omega=(\theta,\phi)$ is a unit vector, and θ,ϕ are the angular spherical coordinates, are normalized in $L^2(S^2)$, where S^2 is the unit sphere [n is a multi-index $n=(l,m)$].

For large orders ($l\gg kr$) in ψ_n and $\operatorname{Re}\psi_n$ it is known[20] that

$$\begin{aligned}\psi_n(x)&\sim -i(2l-1)!!(kr)^{-l-1}\,Y_n(\omega),\\ \operatorname{Re}\psi_n(x)&\sim[(2l+1)!!]^{-1}(kr)^l\,Y_n(\omega).\end{aligned} \tag{45}$$

For large orders l the spherical waves are essentially a perturbation of the basis $Y_n(\omega)$ by a power of kr. This is the promised motivation for the choice of the model example in (41).

In the numerical data given below we have also included the spherical harmonics Y_n and the functions

$$\chi_n(x)=(kr)^{-l-1}\,Y_n(\omega), \tag{46}$$

TABLE I. The condition number κ as a function of different truncation sizes and eccentricities for the model problem [see (41)]. The corresponding condition number κ for the normalized functions $\phi_m\cdot(\phi_m,\phi_m)^{-1/2}$ is given in parentheses.

	Truncation size							
Eccentricity	5		10		20		40	
$q=0.1$	6	(4)	60	(40)	8×10^3	(5×10^3)	2×10^8	(1×10^8)
$q=1/3$	1×10^2	(80)	7×10^4	(4×10^4)	3×10^{10}	(2×10^{10})	$>10^{16}$	$(>10^{16})$
$q=1$	8×10^3	(5×10^3)	1×10^9	(6×10^8)	$>10^{16}$	$(>10^{16})$	$>10^{16}$	$(>10^{16})$

which are solutions of the equation $\Delta u = 0$ in Ω. The factor k in (46) was used in order for the factor kr to be dimensionless.

The Gram matrix for these four systems has matrix elements, which are double integrals over the unit sphere. We assume that the equation of the surface Γ can be written as $s = p(\omega)$, where $\omega \in S^2$, and p is a smooth invertible function, so that $\omega = p^{-1}(s)$. In our calculations the functions (44) and (46) were considered on Γ, i.e., as function of s, where $r = |s|$, $x = s$ on the surface Γ. If the bodies are axially symmetric, then the matrix elements of the Gramians can be written as single integrals in θ, and for simplicity we choose the surface of a spheroid, i.e.,

$$r(\theta) = (\sin^2\theta/a^2 + \cos^2\theta/b^2)^{-1/2}, \tag{47}$$

where a and b are the semiaxes of the spheroid (θ is the polar angle, so that b is the semiaxis along the axis of symmetry). The mirror symmetry $r(\theta) = r(\pi - \theta)$ implies that l even and l odd do not couple. Thus the elements of the Gram matrix are zeroes if $l + l'$ is odd. In this case we can change the enumeration of the columns and rows in the matrix so that it becomes a block diagonal matrix with two blocks. The size of the first block, which corresponds to the rows with even numbers, is $(l_{\max} + 1)/2$ if $l_{\max}$ is odd, and $l_{\max}/2 + 1$ if $l_{\max}$ is even. The size of the second block, which corresponds to the row with odd numbers, is $(l_{\max} + 1)/2$ if $l_{\max}$ is odd, and $l_{\max}/2$ if $l_{\max}$ is even.

The numerical computations seem to indicate that neither of the systems $\{\psi_n\}$, $\{\mathrm{Re}\,\psi_n\}$, or $\{\chi_n\}$ forms a Riesz basis of $H_0 = L^2(\Gamma)$. However, $\{Y_n(p^{-1}(s))\}$ forms a Riesz basis of H_0 as has been proven earlier.[11] It is seen from Table II that the spherical waves $\{\psi_n\}$, $\{\mathrm{Re}\,\psi_n\}$, and $\{\chi_n\}$ are not good for expansions in the sense that the condition number of the Gram matrix grows as the truncation size increases. Indeed, in this more realistic example the tendencies (1)–(3) discussed above for the model problem are valid, together with the following additional observation:

(4) The systems $\{\psi_n\}$ and $\{\chi_n\}$ have smaller condition number than $\{\mathrm{Re}\,\psi_n\}$.

The numerical data seems to indicate that the normalized functions should be used for expansions of the surface field since the corresponding Gram matrix has a smaller condition number. Furthermore, there is an indication that for high truncations the normalized systems $\{\psi_n\}$ and $\{\chi_n\}$ are better than $\{\mathrm{Re}\,\psi_n\}$. However, the difference is not very considerable. A large condition number means that the Gram matrix is difficult to invert numerically. It also means numerical instability, i.e., strong dependence of the numerical results on the roundoff errors and errors in the data.

It should be noted that the Gram matrix is identical to a Q matrix[6] in the T-matrix scheme for a special choice of expansion functions. Thus, some of the properties mentioned above might appear within this scheme for this special choice of the expansion functions. It should also be noted that when the T-matrix scheme is used to compute the scattered field, additional operators enter, which tend to improve the situation. However, a discussion of these aspects requires further investigation.

4. CONCLUDING REMARKS

There are several questions, raised by the T-matrix approach to scattering, which require further study. We conclude by giving a short list of such questions.

(1) Try the system

$$v_n(x) = \int_\Gamma \frac{\exp(ik\,|x - s|)}{4\pi|x - s|}\,\phi_n(s)\,dS, \quad x \in \Omega,$$

of outgoing waves for calculations. Here the system $\{\phi_n\}$ is a complete system in $H_0 = L^2(\Gamma)$. If the system $\{\phi_n\}$ forms a Riesz basis of $H_{-1/2}$, then the system $\{v_n\}$ on Γ forms a Riesz basis of H_0. This was established in Ref. 11. From the results in Ref. 11 it follows that any solution of the problem (1)–(3) can be represented by the series $u = \sum_{n=1}^{\infty} c_n v_n(x)$,

TABLE II. The condition number κ as a function of truncation sizes and eccentricities for three different spherical waves $\{\psi_n\}$, $\{\mathrm{Re}\,\psi_n\}$, $\{\chi_n\}$, and the spherical harmonics $\{Y_n\}$. The corresponding condition number for the normalized functions is given in parentheses. $m = 0$ in all cases.

	5 even	5 odd	9 even	9 odd	19 even	19 odd
$ka = 4$						
$kb = 2$						
ψ_n	30 (3)	400 (4)	2×10^7 (30)	1×10^9 (50)	$>10^{16}$ (3×10^4)	$>10^{16}$ (6×10^4)
$\mathrm{Re}\,\psi_n$	30 (20)	400 (10)	5×10^6 (200)	2×10^8 (400)	$>10^{16}$ (1×10^6)	$>10^{16}$ (3×10^6)
χ_n	1×10^3 (5)	1×10^3 (8)	2×10^6 (50)	2×10^6 (100)	1×10^{14} (4×10^4)	1×10^{14} (1×10^5)
Y_n	3 (3)	3 (3)	4 (4)	4 (4)	4 (4)	4 (4)
$ka = 6$						
$kb = 2$						
ψ_n	30 (3)	40 (5)	2×10^7 (40)	1×10^9 (90)	$>10^{16}$ (1×10^5)	$>10^{16}$ (3×10^5)
$\mathrm{Re}\,\psi_n$	400 (400)	20 (80)	4×10^4 (500)	8×10^5 (1×10^3)	$>10^{16}$ (1×10^8)	$>10^{16}$ (3×10^8)
χ_n	2×10^4 (6)	2×10^4 (10)	3×10^6 (100)	3×10^6 (200)	5×10^{14} (2×10^5)	4×10^{14} (4×10^5)
Y_n	7 (7)	6 (6)	9 (9)	9 (9)	10 (10)	10 (10)
$ka = 10$						
$kb = 2$						
ψ_n	30 (3)	300 (5)	2×10^7 (50)	1×10^9 (100)	$>10^{16}$ (2×10^5)	$>10^{16}$ (4×10^5)
$\mathrm{Re}\,\psi_n$	30 (30)	3 (2)	60 (30)	600 (200)	5×10^{14} (8×10^8)	7×10^{15} (2×10^9)
χ_n	3×10^3 (6)	2×10^3 (10)	5×10^6 (100)	4×10^6 (300)	1×10^{14} (3×10^5)	7×10^{14} (8×10^5)
Y_n	20 (20)	10 (10)	30 (30)	30 (30)	40 (40)	40 (40)

which converges in Ω up to the boundary. Indeed, assume (without loss of generality) that k^2 is not an eigenvalue of the Dirichlet Laplacian in $\mathscr{D}$. Then the solution to the problem (1)–(3) can be written as

$$u(x) = \int_\Gamma \frac{\exp(ik|x-s|)}{4\pi|x-s|}\sigma(s)\,dS,$$

where σ is the unique solution to the equation

$$\int_\Gamma \frac{\exp(ik|s'-s|)}{4\pi|s'-s|}\sigma(s')\,dS = f(s).$$

If $\{\phi_n\}$ forms a basis of $L^2(\Gamma)$, then $\sigma = \Sigma_{n=1}^\infty c_n \phi_n$, where the series converges in $L^2(\Gamma)$. Therefore $u(x) = \Sigma_{n=1}^\infty c_n v_n(x)$, where the series converges uniformly in the closure of Ω. This was the reason for suggesting the system $\{v_n\}$ instead of the usual outgoing waves (44), which do not seem to form a Riesz basis on nonspherical surfaces. The other reason for choosing $\{v_n\}$ was that since the expansion of the solutions to Helmholtz' equation in the exterior domain in the functions v_n converges up to the boundary, no difficulties with the Rayleigh hypothesis arise.

(2) It was noted in Sec. 3.2 that the Gram matrices correspond (for a particular choice of expansion systems) to a Q matrix. More extensive numerical experiments concerning the condition number for various matrices $a_{ij} \equiv (\phi_i, \bar{\psi}_j)$ (i.e., Q matrices) are called for. This would provide a better basis for judging the performance of specific choices ϕ_i and ψ_j and thus provide a more detailed answer to Q5.

(3) In the present article we have concentrated on "the null field equations" [5] [i.e., (7), (11), etc.] and the question of obtaining a solution on the surface Γ. In the T-matrix scheme one, furthermore, computes the (truncated) transition matrix $(T)_m$ of the form

$$(T)_m = (Q')_m \cdot [(Q'')_m]^{-1}, \tag{48}$$

where the $m \times m$ matrices $(Q')_m$ and $(Q'')_m$ are similar to the Q^1 and Q^2 matrices in Appendix B. The exact (infinite) T matrix is independent of the expansion systems used on Γ. However, the approximate truncated matrix, computed according to (48), does contain such a dependence. It is of interest to investigate the rate of convergence of truncated forms like (48) to the true, infinite transition matrix for the scatterer in question. It is then of interest to exploit general constraints on the scattering matrix such as unitarity and symmetry (see, e.g., Ref. 7 and the contribution by P. C. Waterman in Ref. 5).

(4) Extend the discussion of Ref. 11 and the present work to the case of a penetrable scatterer. Of particular relevance here is the relation between the convergence rates in the expansion used for the surface fields and their normal derivatives (one aspect of this relation is treated in Appendix B).

(5) Study the convergence questions for the T-matrix scheme for scattering from obstacles with noncompact (infinite) boundaries. In this context the work in Ref. 21 will be useful. In Ref. 21 the scattering problem was formulated and solved for domains with noncompact boundaries. For the boundaries, which are locally Liapunov and such that, outside of a sphere of arbitrarily large but fixed radius, the points of the boundary can be seen from a point located outside the domain $\mathscr{D}$ (in this case infinite), it was proved in Ref. 21 that the Schrödinger operator with decreasing real-valued potential has no positive discrete spectrum and the radiation condition selects a unique solution to the Dirichlet boundary value problem. The case of the third boundary condition was also treated. Furthermore, the existence, uniqueness, and properties of the resolvent kernel G of the Schrödinger operator were studied in detail. In particular, global estimates of $G(x,y,k)$ and its derivatives, uniform in $a \leqslant k \leqslant C$, $0 < a < C < \infty$, were obtained for $|x-y| \to 0$ and $|x-y| \to \infty$. It was proved that the limit $G(x,y,k+i\epsilon)$ as $\epsilon \to 0$, $\epsilon > 0$, does exist and is attained uniformly in $a \leqslant k \leqslant C$. This was done for the boundaries Γ for which $\rho(s,\Gamma_0) \times (1+|s|^\alpha) \to 0$ as $|s| \to \infty$, $s \in \Gamma$. Here $\alpha > n$, where n is the dimension of the space, and Γ_0 is the boundary of the "canonical" domain (the boundary of a cone if $n > 2$, and of a wedge in the two-dimensional case). It was proved[21] that $G(x,y,k) = (e^{ikr}/4\pi r)\, u(\nu,y,k)\cdot[1+o(1)]$ as $|x| = r \to \infty$, $xr^{-1} = \nu$, where the functions $u(\nu,y,k)$ are the solutions of the scattering problem in the sense that they solve the Schrödinger equation and vanish on Γ. Furthermore, it was shown that an arbitrary function $f \in L^2(\mathscr{D})$ can be expanded in a Fourier integral in functions u and a Fourier series corresponding to the negative discrete spectrum of the Schrödinger operator. If the potential is equal to zero, then the Fourier series part of the expansion is absent. The wave operators were constructed in Ref. 21 with the help of the eigenfunction expansions.

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APPENDIX A: SOME RESULTS FROM LINEAR FUNCTIONAL ANALYSIS

1. The gap of subspaces of a Hilbert space and a condition for invertibility of the mixed Gram matrix (ϕ_i, ψ_j)

Let H_1 and H_2 be (closed) subspaces of a Hilbert space H. Then the gap of H_1 and H_2 is defined as

$$\theta(H_1, H_2) = \| P_1 - P_2 \|,$$

where P_1 and P_2 are the orthoprojections onto H_1 and H_2, respectively. Clearly, $0 \leqslant \theta \leqslant 1$, $\theta(H_1,H_2) = \theta(H_2,H_1)$. It can be proved[14] that

$$\theta(H_1,H_2) = \max\left\{ \sup_{\substack{\|x\|=1\\ x\in H_1}} \|(I-P_2)x\|, \quad \sup_{\substack{\|x\|=1\\ x\in H_2}} \|(I-P_1)x\| \right\}.$$

The following facts hold (Ref. 14, pp. 252–60).

Lemma 1: Let G_n and H_n be n-dimensional subspaces of a Hilbert space H and $\theta(G_n, H_n) < 1$. Then G_n and H_n

have orthogonal bases $u_1,\dots,u_n$ and $v_1,\dots v_n$, respectively, and $(u_i, v_j) = \beta_i\,\delta_{ij}$, $1\leqslant i,j\leqslant n$, where

$$\delta_{ij} = \begin{cases}1, & i=j,\\ 0, & i\neq j,\end{cases} \quad \{1-\theta^2(G_n, H_n)\}^{1/2}\leqslant \beta_i \leqslant 1.$$

Lemma 2: Let $\{\phi_j\}$ and $\{\psi_j\}$, $1\leqslant j\leqslant m$, be two sets of linearly independent elements of H. Let $0<\lambda_m$ and $0<\mu_m$ denote the smallest eigenvalues of the matrices (ϕ_i, ϕ_j) and (ψ_i, ψ_j), $1\leqslant i,j\leqslant m$, respectively. Let G_m and H_n be linear spans of $\phi_1,\dots,\phi_m$ and $\psi_1,\dots,\psi_m$, respectively, and $A_m = (\phi_i, \psi_j)$, $1\leqslant i,j\leqslant m$. Let $\theta(G_m, H_m)<1$. Then A_m is invertible and

$$\|A_m^{-1}\|\leqslant \alpha_m/(\lambda_m\,\mu_m)^{1/2},$$

where

$$\alpha_m = [1-\theta^2(G_m, H_m)]^{1/2}.$$

2. Minimal systems

A system of elements is called *minimal* if none of the elements belongs to the closure of the linear span of the others. A minimal system $\{\phi_j\}$ is called *strongly minimal* if $\lim_{m\to\infty}\lambda_m = \lambda>0$, where λ_m is the minimal eigenvalue of the Gram matrix $\phi_{ij} = (\phi_i, \phi_j)$, $1\leqslant i,j\leqslant m$. A system $\{\tilde\phi_j\}$ is called biorthogonal to the system $\{\phi_j\}$ if $(\tilde\phi_j, \phi_i) = \delta_{ij}$. The biorthogonal system $\{\tilde\phi_j\}$ is uniquely defined iff the system $\{\phi_j\}$ is minimal.

A system $\{\phi_j\}$ of linearly independent elements of a Hilbert space H is called *closed* in this space iff for $f\in H$ the conditions $(f, \phi_j) = 0$, $\forall j$, imply that $f=0$.

A system $\{\phi_j\}$ of linearly independent elements of H is called *complete* in H iff for any $f\in H$ and any given positive number $\epsilon>0$ one can find an element $\Sigma_{j=1}^{m(\epsilon)} c_j\,\phi_j$ such that $\|f-\Sigma_{j=1}^{m(\epsilon)} c_j\,\phi_j\|<\epsilon$. Here the constants c_j and the number $m(\epsilon)$ depend on ϵ and f.

A system $\{\phi_j\}$ can be complete but not form a basis of H (see subsection 3 below the definitions of bases).

Example: $H = L^2([0,1])$, $\phi_j = x^j$, $0\leqslant j<\infty$. This system is complete in H, but is not a basis of H. Completeness follows from the Weierstrass approximation theorem. The fact that the system $\{x^j\}$ is not a basis of H can also be easily explained. Suppose that $\{x^j\}$ is a basis of H. Then (see subsection 3 below) for any $f\in H$ the series $f = \Sigma_{j=0}^{\infty} c_j\,x^j$ converges in $L^2([0,1])$. Therefore, f is analytic in $|x|<1$ and cannot be an arbitrary element of H. In fact, from Müntz's theorem[16] it follows that the system $\{\phi_j\}$ is not even minimal (every Schauder's basis is a minimal system). The Müntz's theorem says that the system $\{x^{p_j}\}$, $p_0 = 0$, $0<p_1<p_2<\cdots$ is complete in $L^2([0,1])$ if there exists an infinite subsequence p_j' such that $\Sigma_{j=1}^{\infty}(1/p_j') = \infty$.

3. Bases

A system $\{\phi_j\}$ is called a *Schauder basis* of a Banach space X if any element $x\in X$ can be uniquely represented as $x = \Sigma_{j=1}^{\infty} c_j\,\phi_j$, where the series converges in the norm of X. A system $\{\phi_j\}$ is called a *Riesz basis* of a Hilbert space H iff $\phi_j = Th_j$, where $\{h_j\}$ is an orthonormal basis of H and T is a linear bounded and boundedly invertible operator (i.e., T^{-1} is bounded and defined on all of H). A system $\{\tilde\phi_j\}$ biorthogonal to a basis $\{\phi_j\}$ of H is also a basis of H.

A complete system $\{\phi_j\}$ in H is a Riesz basis of H iff the matrix $\phi_{ij} = (\phi_i, \phi_j)$, $1\leqslant i,j<\infty$, generates a bounded and boundedly invertible operator on l^2.

A complete system $\{\phi_j\}$ in H is a Riesz basis of H iff there exist positive constants a_1 and a_2 such that

$$a_1^2\sum_{j=1}^{m}|c_j|^2\leqslant\left\|\sum_{j=1}^{m} c_j\,\phi_j\right\|^2\leqslant a_2^2\sum_{j=1}^{m}|c_j|^2,$$

for any m and any constants c_j, $1\leqslant j\leqslant m$. If $\{\phi_j\}$ is a Riesz basis, then $\sup_{1\leqslant j<\infty}\|\phi_j\|\leqslant a_2$, $\inf_{1\leqslant j<\infty}\|\phi_j\|\geqslant a_1$ and similar inequalities hold for $\|\tilde\phi_j\|$. In particular, $\sup_{1\leqslant j<\infty}\|\tilde\phi_j\|<\infty$. These results can be found, e.g., in Refs. 16, 17, and 19. In Ref. 15 the notion of the Riesz basis with brackets is applied to some non-self-adjoint integral equations arising in scattering theory.

4. Tests for boundedness and compactness of a linear operator on l^2

Let (a_{ij}), $1\leqslant i,j<\infty$, be a matrix which is considered as a linear operator A on l^2. When is A bounded and when is A compact?

$$(Ax)_i = a_{ij}\,x_j.$$

Here and below we sum over the repeated indices:

$$\|Ax\|^2 = a_{ij}\,x_j\,\bar a_{ik}\,\bar x_k\leqslant|a_{ij}\,\bar a_{ik}|\,\frac{|x_k|^2+|x_j|^2}{2}$$

$$\leqslant\sup_{1\leqslant k<\infty}\sum_{j=1}^{\infty}|a_{ij}\,a_{ik}|\,\|x\|^2.$$

Therefore,

$$\|A\|\leqslant\sup_{1\leqslant k<\infty}\left(\sum_{j=1}^{\infty}\sum_{i=1}^{\infty}|a_{ij}\,a_{ik}|\right)^{1/2}. \tag{A1}$$

The operator A is compact if

$$\sup_{1\leqslant k<\infty}\left(\sum_{j=1}^{\infty}\sum_{i=1}^{\infty}|a_{ij}\,a_{ik}|\right)^{1/2}<\infty$$

and

$$\sup_{1\leqslant k<\infty}\sum_{j=1}^{\infty}\sum_{i=N}^{\infty}|a_{ij}\,a_{ik}|\to 0,\quad N\to\infty. \tag{A2}$$

Lemma (Schur): Let $a_{ij} = \bar a_{ji}$ and $\sup_i\Sigma_j|a_{ij}|\leqslant M$. Then $\|A\|\leqslant M$, A: $l^2\to l^2$.

Proof: It suffices to prove that $|(Ax, x)|\leqslant M\|x\|^2$. One has

$$|(Ax,x)|\leqslant\left|\sum_{i,j}a_{ij}\,x_j\,\bar x_i\right|\leqslant\sum_{i,j}|a_{ij}|\,\frac{|x_i|^2+|x_j|^2}{2}$$

$$=\sum_{i,j}|a_{ij}|\,|x_i|^2\leqslant M\|x\|^2.$$

5. Spaces with negative norms[13]

Let H_+ and H be Hilbert spaces such that $H_+\subset H$ and H_+ is dense in H. Let $u\in H_+$, $f\in H$. Consider the completion H_- of H in the norm

$$\|f\|_- = \sup_{\substack{u\neq 0\\ u\in H_+}} [|(f,u)|/\|u\|_+],$$

where $\|\cdot\|_+$ denotes the norm in H_+ and (f, u) denotes the inner product in H. The space H_- is a Hilbert space, $H_+ \subset H \subset H_-$, and H is dense in H_-.

6. Bessel and Riesz–Fischer systems: Interpolation in Hilbert space

The basic Eqs. (7) can be considered as an interpolation problem in the Hilbert space H [$H = H_0 = L^2(\Gamma)$ in our case], i.e., the problem $(h, \psi_n) = f_n$, $n = 1,2,\cdots$.

Definition 1: A system $\{\psi_n\}$ is called a *Bessel system* if $\Sigma_{n=1}^{\infty} |(h, \psi_n)|^2 < \infty$, whenever $h \in H$.

Definition 2: A system $\{\psi_n\}$ is called a *Riesz–Fischer system* if the problem

$$(h, \psi_n) = f_n, \quad n = 1,2,3,\cdots, \tag{A3}$$

is solvable whenever $\{f_n\} \in l^2$.

The set of sequences $\{(h, \psi_n)\}$, $n \geqslant 1$, $h \in H$, is called the moment space M of $\{\psi_n\}$. The questions of interest are:

(1) When does a sequence $\{f_n\} \in M$? That is, when is the problem $(h, \psi_n) = f_n$, $n \geqslant 1$, solvable?

(2) Is the solution unique?

(3) How to construct the solution?

The answer to question (1) is given by

Proposition 1: In order that (A3) be solvable and $\|h\| \leqslant C$ it is necessary and sufficient that

$$\left|\sum_{n=1}^{m} a_n \bar{f}_n\right| \leqslant C \left\|\sum_{n=1}^{m} a_n \psi_n\right\|$$

for any m and any scalars a_n.

The answer to question (2) was already given: The solution of the problem (A3) is unique iff the system $\{\psi_n\}$ is closed in H. The following facts are useful[19]:

Proposition 2: If (A3) is solvable, then it has a unique solution of minimal norm.

Proposition 3: The solution of

$$(h, \psi_n) = f_n, \quad n \leqslant m, \tag{A4}$$

of minimal norm always exists, is unique, and can be found by the formula

$$h_m = -[\det(\psi_i, \psi_j)]^{-1} \times \det\begin{pmatrix} 0 & \psi_1 & \cdots & \psi_m \\ f_1 & (\psi_1, \psi_1) & \cdots & (\psi_1, \psi_m) \\ \vdots & & & \\ f_m & (\psi_m, \psi_1) & \cdots & (\psi_m, \psi_m) \end{pmatrix}. \tag{A5}$$

Moreover, if (A3) is solvable and h is its unique solution of minimal norm, then

$$\|h_m - h\| \to 0, \quad m \to \infty. \tag{A6}$$

APPENDIX B: DISCUSSION OF SOME EXPANSIONS OCCURRING IN THE T-MATRIX SCHEME FOR A PENETRABLE SCATTERER

Using the Green's theorem, one obtains the identity

$$0 = \int_\Gamma \left(\operatorname{Re}\psi_n \frac{\partial u_+}{\partial N_s} - u_+ \frac{\partial \operatorname{Re}\psi_n}{\partial N_s}\right) dS, \quad \forall n, \tag{B1}$$

where $+$ denotes the limit value from the interior [see (44) for the definition of $\operatorname{Re}\psi_n$]. Assuming that the following series converge in $L^2(\Gamma)$,

$$u_+ = \sum_n c_n^{(1)} \psi_n, \tag{B2}$$

$$\frac{\partial u_+}{\partial N_s} = \sum_n d_n^{(1)} \frac{\partial \psi_n}{\partial N_s}, \tag{B3}$$

one substitutes the series in (B1) to obtain

$$0 = \sum_{n'} \left\{ d_{n'}^{(1)} \int_\Gamma \operatorname{Re}\psi_n \frac{\partial \psi_{n'}}{\partial N_s} dS - c_{n'}^{(1)} \int_\Gamma \psi_{n'} \frac{\partial \operatorname{Re}\psi_n}{\partial N_s} dS \right\}, \quad \forall n. \tag{B4}$$

Truncating the series and using the first m equations in (B4), one obtains a linear system, which can be solved for $c_n^{(1)}$ or $d_n^{(1)}$.

In the case when ψ_n and $\operatorname{Re}\psi_n$ are defined as in (44), it follows from the formula

$$\int_\Gamma \left[\operatorname{Re}\psi_n \frac{\partial \psi_{n'}}{\partial N} - \psi_{n'} \frac{\partial \operatorname{Re}\psi_n}{\partial N}\right] dS = \lambda \delta_{nn'} \tag{B5}$$

that the truncated linear system can be written as

$$Q^{(1)} \mathbf{d}^{(1)} - (Q^{(1)} - \lambda I)\, \mathbf{c}^{(1)} = 0, \tag{B6}$$

where $\mathbf{d}^{(1)} = (d_1^1, \ldots, d_m^1)$, $\mathbf{c}^{(1)} = (c_1^1, \ldots, c_m^1)$, and

$$Q_{nn'}^{(1)} \equiv \int_\Gamma \operatorname{Re}\psi_n \frac{\partial \psi_{n'}}{\partial N_s} dS, \quad n,n' \leqslant m \tag{B7}$$

(λ is a known scalar, depending on the normalization of ψ_n and $\operatorname{Re}\psi_n$). Term by term differentiation of (B2) would imply $\mathbf{c}^{(1)} = \mathbf{d}^{(1)}$, which is not consistent with (B6). That termwise differentiation can*not* be used to obtain $\mathbf{d}$ [by taking $d_n^{(1)} = c_n^{(1)}$ in (B2)–(B3)] is most easily seen from the following example in which Γ is a sphere of radius a and in which one keeps only one term in the series (B2), so that the questions about convergence of the series are irrelevant. Take $u_+ = h_n^{(1)}(ka)\, Y_n(\omega)$. Since $(\nabla^2 + k^2) u = 0$ for $|x| \leqslant a$ and $u|_{r=a} = h_n^{(1)}(ka)\, Y_n(\omega)$, one finds that $u(x) = [h_n^{(1)}(ka)/j_n(ka)]\, j_n(kr)\, Y_n(\omega)$ [we assume that $j_n(ka) \neq 0$]. Therefore,

$$\left.\frac{\partial u_+}{\partial N}\right|_{r=a} = \frac{kh_n^{(1)}(ka)}{j_n(ka)} j_n'(ka)\, Y_n(\omega) \neq \left.\frac{\partial}{\partial N_s} h_n^{(1)}(kr)\, Y_n(\omega)\right|_{r=a} = kh_n^{(1)\prime}(ka)\, Y_n(\omega).$$

Indeed,

$$h_n^{(1)}(ka) j_n'(ka)/j_n(ka) - h_n^{(1)\prime}(ka) = [j_n(ka)]^{-1} [h_n^{(1)}(ka) j_n'(ka) - h_n^{(1)\prime}(ka) j_n(ka)] \neq 0.$$

The numerator is the Wronskian of $h_n^{(1)}$ and j_n and is not zero. The general explanation is that even if one can continue the series (B2) analytically inside $\mathscr{D}$ in a neighbourhood of Γ, this continuation *will be different from* the solution u of the problem

$$(\nabla^2 + k^2) u = 0 \quad \text{in } \mathscr{D}, \quad u|_\Gamma = u_+, \tag{B8}$$

so that $\partial u_+/\partial N_s \neq \partial w/\partial N_s$ on Γ, where w denotes the analytic continuation of the series (B2) in $\mathscr{D}$. Indeed, $u_+ = w$ on

Γ, and if $\partial u_+/\partial N = \partial w/\partial N$ on Γ, then $u \equiv w$ in $\mathscr{D}$ by the uniqueness of the solution to the Cauchy problem for Helmholtz' equation. But this leads to a contradiction since w is singular at the origin ($0 \in \mathscr{D}$).

If, instead of (B2) and (B3), we consider the expansions

$$u_+ = \sum_n c_n^{(2)} \operatorname{Re} \psi_n, \tag{B9}$$

$$\frac{\partial u_+}{\partial N} = \sum_n d_n^{(2)} \frac{\partial \operatorname{Re} \psi_n}{\partial N_s}, \tag{B10}$$

then the truncated matrix equation analogous to (B6) reads

$$Q^{(2)}\mathbf{d}_n^{(2)} = Q^{(2)}\mathbf{c}^{(2)}, \tag{B11}$$

where

$$Q_{nn'}^{(2)} \equiv \int_\Gamma \operatorname{Re} \psi_n \frac{\partial \operatorname{Re} \psi_{n'}}{\partial N_s} dS. \tag{B12}$$

Thus, assuming that $\{Q_{nn'}^{(2)}\}, n,n' \leqslant m$, is invertible, we obtain

$$\mathbf{c}^{(2)} = \mathbf{d}^{(2)} \tag{B13}$$

(this result is used in the T-matrix approach to scattering from a permeable body[6,7]).

A relevant fact of more general nature is the following lemma.

Lemma: Let

$$(\nabla^2 + k^2) u = 0 \quad \text{in } \mathscr{D}, \ k>0,$$

$$(\nabla^2 + k^2) \phi_j = 0 \quad \text{in } \mathscr{D}, \ 1 \leqslant j \leqslant m,$$

$$u_m = \sum_{j=1}^m c_j^{(m)} \phi_j, \quad \frac{\partial u_m}{\partial N} = \sum_{j=1}^m c_j^{(m)} \frac{\partial \phi_j}{\partial N}.$$

Assume that

$$\left\{(\nabla^2 + k^2) u = 0, \quad \frac{\partial u}{\partial N_s}\bigg|_\Gamma = 0\right\} \Rightarrow u \equiv 0 \quad \text{in } \mathscr{D}$$

(so that the Green's function G_N for the interior Neumann problem exists and is unique) and that the $\{c_j^{(m)}\}, j \leqslant m$, have been determined so that [where $\|\cdot\|$ is the norm in $H_0 = L^2(\Gamma)$]

$$\left\|\frac{\partial u}{\partial N_s} - \frac{\partial u_m}{\partial N_s}\right\| < \epsilon. \tag{B14}$$

Then

$$\| u - u_m \| < c\epsilon. \tag{B15}$$

Here and below c denotes various constants depending on Γ.

Proof: Let $u - u_m \equiv v$. Then $(\nabla^2 + k^2) v = 0$ in $\mathscr{D}$ and $\| \partial v/\partial N \| < \epsilon$. We have

$$v(x) = \int_\Gamma \left[G_N(x, s') \frac{\partial v}{\partial N'_s} - v \frac{\partial G_N(x, s')}{\partial N'_s}\right] dS'$$

$$= \int_\Gamma G_N(x, s') \frac{\partial v}{\partial N'_s} dS', \quad x \in \mathscr{D},$$

and also

$$v(s) = \int_\Gamma G_N(s, s') \frac{\partial v}{\partial N'_s} dS', \quad s \in \Gamma.$$

The following estimate is known[1]:

$$| G_N(s, s')| \leqslant c/| s - s'|.$$

With $h \equiv \partial v/\partial N$ we then have

$$|v(s)| \leqslant c \int_\Gamma \frac{|h| \, dS'}{|s - s'|},$$

which implies

$$\| v\| \leqslant c\epsilon$$

since the operator S: $H_0 \to H_0$ $[H_0 = L^2(\Gamma)]$,

$$(Sh)(s) \equiv \int_\Gamma \frac{h(s') \, dS'}{|s - s'|},$$

is bounded. In fact, also S: $H_0 \to H_1$ is bounded. Therefore,

$$\left\|\frac{\partial v}{\partial s}\right\| \leqslant c\epsilon,$$

where $\partial v/\partial s$ is any tangential derivative of v. In the above it was essential that the $c_j^{(m)}$, $1 \leqslant j \leqslant m$, were determined so that (B14) was valid. If, instead the $c_j^{(m)}, j \leqslant m$, are chosen so that

$$\| u - u_m \| < \epsilon \tag{B16}$$

and if we assume in this case that

$$\{(\nabla^2 + k^2) u = 0, \ u|_\Gamma = 0\} \Rightarrow u \equiv 0 \quad \text{in } \mathscr{D},$$

(so that the Green's function G_D for the interior Dirichlet problem exists and is unique), we have

$$\frac{\partial}{\partial N_0} v(x) = - \frac{\partial}{\partial N_0} \int_\Gamma v(s) \frac{\partial G_D(x, s)}{\partial N_s} dS, \quad x \in \mathscr{D},$$

where N_0 is a direction which coincides with the normal to Γ on Γ. However, when we let x approach Γ, we do not obtain a bounded operator on H_0 in the present case. In fact, *the estimate* (B15) *does not imply*

$$\int_\Gamma \left| \frac{\partial u}{\partial N_s} - \sum_{j=1}^m c_j^{(m)} \frac{\partial \phi_j}{\partial N_s}\right|^2 dS \leqslant \delta(\epsilon), \quad \delta(\epsilon) \underset{\epsilon \to 0}{\to} 0, \tag{B17}$$

even in the case $u|_\Gamma = f \in C^\infty$. *Here* u *is the solution to the problem*

$$(\nabla^2 + k^2) u = 0 \quad \text{in } \mathscr{D}, \quad u|_\Gamma = f, \tag{B18}$$

and ϕ_j *solve the equation*

$$(\nabla^2 + k^2) \phi_j = 0 \quad \text{in } \mathscr{D}. \tag{B19}$$

Proof: If we consider the function $f_\epsilon \in L^2(\Gamma)$, $\|f_\epsilon\| < \epsilon$, then $\| h_\epsilon - \Sigma_{j=1}^m c_j^{(m)} \phi_j\| < 2\epsilon$, where $h_\epsilon = f + f_\epsilon$. Let u_ϵ denote the solution of (B18). One can see that $\| \partial u_\epsilon/\partial N - \Sigma_{j=1}^m (c_j^{(m)} \partial \phi_j/\partial N)\|$ can be as large as one wishes if f_ϵ is chosen appropriately. In fact, $\partial u_\epsilon/\partial N$ can be even not defined on Γ. To see this, one can take $k = 0$ and $\mathscr{D}$ to be a circle of radius 1. Then

$$\left.\begin{aligned} u_\epsilon &= \sum_{n=-\infty}^\infty h_{\epsilon n} r^{|n|} e^{in\phi}, \\ h_{\epsilon n} &= \frac{1}{2\pi} \int_{-\pi}^\pi e^{-in\phi} h_\epsilon(\phi) \, d\phi, \end{aligned}\right\} \quad r<1,$$

$$\frac{\partial u_\epsilon}{\partial N} = \frac{\partial u_\epsilon}{\partial r} = \sum_{\substack{n=-\infty \\ n \neq 0}}^\infty |n| h_{\epsilon n} r^{|n|-1} e^{in\phi}. \tag{B20}$$

If $\Sigma_{n=-\infty}^\infty |nh_{\epsilon n}| = \infty$, the function (B20) has no limit in $L^2(\Gamma)$ as $r \to 1 - 0$. If $\Sigma_{n=-\infty}^\infty |nh_{\epsilon n}|^2 = c^2 < \infty$, then the limit does exist and $\| \partial u_\epsilon/\partial N \| = 2\pi c$ can be as large as one wants if f_ϵ is chosen appropriately.

APPENDIX C: ABOUT PROJECTION METHODS

1. Convergence of projection methods

Let A be a linear bounded and boundedly invertible operator from a Hilbert space H onto a Hilbert space G. Let P_m be the orthoprojection onto L_m, where L_m is an m-dimensional subspace of H, $L_{m+1} \supset L_m$, and the sequence of the subspaces L_m is limit dense in H, i.e., for any $h \in H$ the distance from h to L_m goes to zero as $m \to \infty$. Let Q_m be the orthoprojection onto M_m, where M_m is an m-dimensional subspace of G, $M_{m+1} \supset M_m$, and the sequence $\{M_m\}$ is limit dense in G.

Consider the equation

$$Ah = f \tag{C1}$$

and the projection method of its approximate solution

$$Q_m AP_m h_m = Q_m f. \tag{C2}$$

The question of when the following statement is true is then of interest:

Equation (C2) is uniquely solvable for all sufficiently large m and $\| h_m - h \| \to 0, \quad m \to \infty.$ (C3)

Here h_m is the solution of (C2). In the problem described in the Introduction, $h_m = \Sigma_{j=1}^m c_j^{(m)} \phi_j$, and P_m is the orthoprojection in $H = L^2(\Gamma)$ onto the linear span of $\phi_1,\dots,\phi_m$, $G = l^2$, Q_m is the orthoprojection in l^2 onto the linear span of the first m coordinate vectors in l^2, i.e., onto the subspace of the vectors whose components f_n vanish for $n > m$. The following theorem, which is a particular case of a more general result from Ref. 18, p. 91, answers the above question.

Theorem 1: (C3) holds iff

$$\| Q_m AP_m h \| \geqslant c \| P_m h \|, \quad \forall m > m_0, \quad \forall h \in H, \quad c > 0, \tag{C4}$$

and

$$Q_m AP_m H = Q_m G, \quad \forall m > m_0. \tag{C5}$$

Remark 1: If P_m and Q_m are projections onto m-dimensional spaces, where $m = 1,2,\cdots$ (this is the case we are interested in this paper), then (C4) implies (C5), because the operator $Q_m AP_m : P_m H \to Q_m G$ is an injective mapping between two m-dimensional spaces and therefore this mapping is surjective.

Proof: (1) (C3) $\Rightarrow$ (C4)–(C5). If (C3) holds, then (C2) is uniquely solvable for $m > m_0$ and therefore (C5) holds. Furthermore, $(Q_m AP_m)^{-1} Q_m f \to A^{-1} f = h$, $\forall f \in G$. Therefore, $\|(Q_m AP_m)^{-1} Q_m\| \leqslant c < \infty$. Here and below c denotes various positive constants. Thus $\| P_m h \| = \|(Q_m AP_m)^{-1} Q_m Q_m AP_m h \| \leqslant c \| Q_m AP_m h \|$, i.e., (C4) holds. Note that $(Q_m AP_m)^{-1} \cdot Q_m AP_m = I_m$, where I_m is the identity in $P_m H$ (not in all of H).

(2) (C4)–(C5) $\Rightarrow$ (C3). From (C5) it follows that (C2) is uniquely solvable for $m > m_0$. To show that $\| h_m - h \| \to 0$, $m \to \infty$, consider the equalities

$$Q_m A [P_m h + (I - P_m) h] = Q_m f,$$

$$Q_m AP_m h_m = Q_m f,$$

which imply that

$$Q_m AP_m (h_m - P_m h) = Q_m A (I - P_m) h. \tag{C6}$$

Since the sequence of the subspaces L_m is limit dense in H, one has $(I - P_m) h \to 0$, $\forall h \in H$. Therefore, (C6) and (C4) imply that

$$\| h_m - P_m h \| = \| P_m (h_m - P_m h) \| \leqslant c \| Q_m A (I - P_m) h \| \to 0, \quad m \to \infty. \tag{C7}$$

Thus

$$\| h - h_m \| \leqslant \| h - P_m h \| + \| P_m h - h_m \| \to 0, \quad m \to 0. \tag{C8}$$

This completes the proof, which is borrowed from Ref. 18 (see also Ref. 22).

2. Stability of the projection methods

Suppose that (C3) holds for the operator A in (C1).

(1) Will it hold for $A + B$ where $\| B \| < \delta$ and $\delta < 0$ is sufficiently small? The answer is yes.

(2) Will it hold for $A + B$ where B is compact and $A + B$ is boundedly invertible? The answer is yes.

The proofs can be found in Ref. 18. Since they are simple, we give them here for convenience of the reader.

(1) Let $\delta = c - \epsilon$, $\| B \| \leqslant \delta$, where c is the constant in (C4), $0 < \epsilon < c$. Then $\| Q_m (A + B) P_m h \| \geqslant c \| P_m h \| - \delta \| P_m h \| = \epsilon \| P_m h \|$. For the case when Q_m and P_m are finite-dimensional projections onto m-dimensional spaces, Theorem 1 is applicable (see Remark 1). In the general case it is not difficult to show that (C5) holds, i.e., that the operator $Q_m (A + B) P_m : P_m H \to Q_m G$ is invertible:

$$Q_m (A + B) P_m = Q_m AP_m [I_m + (Q_m AP_m)^{-1} Q_m BP_m],$$

and $\|(Q_m AP_m)^{-1} Q_m BP_m \| \leqslant (c - \epsilon)/c < 1$. Therefore, conditions (C4)–(C5) are satisfied by the operator $A + B$ and (C3) holds for the operator $A + B$.

(2) If B is compact then $\|(Q_m AP_m)^{-1} Q_m B - A^{-1} B \| \to 0$, $m \to \infty$, because $(Q_m AP_m)^{-1} Q_m \to A^{-1}$ strongly. If $A + B$ is invertible, then so is $I + A^{-1} B$, and $\| P_m h + A^{-1} BP_m h \| > c_1 \| P_m h \|$. Therefore,

$$\begin{aligned}
&\| Q_m (A + B) P_m h \| \\
&\quad = \| Q_m AP_m [P_m h + (Q_m AP_m)^{-1} Q_m BP_m h] \| \\
&\quad \geqslant c \| P_m h + (Q_m AP_m)^{-1} Q_m BP_m h \| \\
&\quad \geqslant c \| P_m h + A^{-1} BP_m h \| \\
&\qquad - c \| [(Q_m AP_m)^{-1} Q_m B - A^{-1} B] P_m h \| \\
&\quad \geqslant \tfrac{1}{2} cc_1 \| P_m h \|, \quad \forall m > m_0.
\end{aligned}$$

Thus, condition (C4) holds for $A + B$. To check condition (C5), one notes that $Q_m AP_m$ is invertible, $Q_m BP_m$ is compact, and $Q_m AP_m + Q_m BP_m$ is one-to-one by virtue of (C4). By Fredholm's alternative, one concludes that $Q_m (A + B) P_m$ is invertible and (C5) holds.

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Positive-definite self-dual solutions of Einstein's field equations

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We investigate (anti-) self-dual Riemann space-times for diagonal Bianchi types of class A with positive-definite metrics. A general algorithm to find self-dual solutions is presented. Explicit solutions are given for all types of class A.

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I. INTRODUCTION

In a recent paper by Caderni *et al.*[1] an investigation of the integrability conditions of the Einstein equations for self-dual Bianchi space-times of class A was made. These are the Bianchi types I, II, VI_0, VII_0, VIII, and IX. It has been stated that there are no self-dual solutions for Bianchi type II in a pseudo-Riemann space-time. In addition these authors have been unable to find a general integrability condition in the cases of Bianchi type VIII and type IX. Furthermore no explicit solutions for the remaining types have been given.

The discovery of pseudoparticle (instanton) solutions to the Euclidean SU(2) Yang–Mills theory[2] has suggested the possibility that analogous solutions might occur in Einstein's theory of gravitation.[3] Since the Yang–Mills instantons possess self-dual field strength, one likely possibility is that gravitational instantons are characterized by self-dual curvature. Thus it seems to be more appropriate to consider a proper Riemann space-time with signature $(+ + + +)$ as was also done in the paper by Belinskii *et al.*[4] on the self-dual Bianchi type IX solution mentioned by Caderni *et al.*[1]

The aim of this paper is to show that the Einstein equations can be completely integrated for all diagonal (anti-)self-dual Bianchi space-times of class A in a Riemann space-time (with positive-definite metrics). We present new exact (anti-)self-dual solutions which in some cases may be regarded as gravitational instantons, i.e., complete Riemann space-times.

II. DERIVATION OF CURVATURE

Let (M,g,σ) be a four-dimensional Riemannian manifold (signature $+ + + +$) with a metric tensor g and a linear connection σ compatible with g. In choosing a local orthonormal basis σ^μ, we can put the metric for diagonal Bianchi space-times in the form

$$ds^2 = \eta_{\mu\nu}\sigma^\mu\sigma^\nu, \tag{1}$$

where $\eta_{\mu\nu} = (1,1,1,1)$ is the Euclidean metric tensor. We take

$$\sigma^0 = \omega^0 = dt,\ \sigma^i = R_i\omega^i \text{ (no sum)}, \tag{2}$$

where ω^i are time-independent differential one-forms and where the R_i are functions of t only. (Here and henceforth Latin indices will assume the values 1, 2, 3, whereas Greek indices will assume the values 0, 1, 2, 3.) The one-forms obey the relations

$$d\omega^i = -\tfrac{1}{2}C_{kl}{}^i\omega^k\wedge\omega^l,\quad d\sigma^i = -\tfrac{1}{2}\gamma_{\alpha\beta}{}^i\sigma^\alpha\wedge\sigma^\beta, \tag{3}$$

where the $C_{kl}{}^i$ are the structure constants, $\gamma_{\alpha\beta}{}^i$ the connection coefficients, and $\wedge$ denotes the exterior product. The structure constants for the Bianchi types of class A can be written as

$$C_{ik}{}^l = \epsilon_{ikl}n_l, \tag{4}$$

where ϵ_{ijk} is the totally antisymmetric Levi-Cività pseudotensor. We have

n_1	n_2	n_3	
0	0	0	type I
1	0	0	type II
1	−1	0	type VI_0
1	1	0	type VII_0
1	1	−1	type VIII
1	1	1	type IX

By using Cartan's calculus of differential forms[5–7] we can easily calculate the corresponding components of the Ricci tensor $R_{\mu\nu}$. Since we are only interested in vacuum solutions of Einstein's field equations we have

$$R_{\mu\nu} = 0. \tag{5}$$

By requiring that the connection forms $\sigma_{\mu\nu}$ be (anti-)self-dual, i.e.,

$$\sigma_{\mu\nu} = \delta\tilde{\sigma}_{\mu\nu} = \tfrac{1}{2}\delta\epsilon_{\mu\nu\rho\tau}\sigma_{\rho\tau}, \tag{6}$$

it follows that the Riemann tensor $R^\mu{}_{\nu\alpha\beta}$ is (anti-)self-dual;

$$R^\mu{}_{\nu\alpha\beta} = \delta\tilde{R}^\mu{}_{\nu\alpha\beta} = \tfrac{1}{2}\delta\epsilon_{\alpha\beta\gamma\rho}R^\mu{}_\nu{}^{\gamma\rho}, \tag{7}$$

where $\delta = 1$ for self-dual and $\delta = -1$ for anti-self-dual solutions. Taking the trace of this equation, we find that the Ricci tensor $R_{\mu\nu}$ vanishes; hence the (anti-)self-dual space-times automatically satisfy the vacuum Einstein equations.

III. FIELD EQUATIONS AND SOLUTIONS

Caderni *et al.*[1] have been also unsuccessful in their attempts to find a general algorithm for obtaining self-dual solutions. We now present such an algorithm to obtain (anti-)self-dual solutions for all Bianchi types of class A. We first consider the (anti-)self-dual condition (6), as has been first discussed by Eguchi *et al.*[8–11] We obtain

$$\sigma_{0i} = \delta\sigma_{jk}, \tag{8}$$

where i, j, k are in cyclic order. The connection one-forms to be considered are

$$\sigma_{0k} = -H_k\sigma^k, \tag{9a}$$

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$$\sigma_{ik} = -\frac{1}{2}\epsilon_{ikl}\left(\frac{n_i R_i}{R_k R_l} + \frac{n_k R_k}{R_i R_l} - \frac{n_l R_l}{R_i R_k}\right)\sigma^l, \quad (9b)$$

where $H_i = \dot{R}_i/R_i$ are the Hubble parameters. (A dot denotes differentiation with respect to time.) It follows that we are able to reduce Einstein's equations to first-order differential equations, analogous to the Yang–Mills case:

$$(\ln R_i^2)' = \delta\epsilon_{jki}(n_j R_j^2 + n_k R_k^2 - n_i R_i^2), \quad (10)$$

where we have introduced the new time variable η by $dt = R_1R_2R_3\, d\eta$, $(\ )' = d/d\eta$.

The linear combination of Eqs. (10) gives

$$(\ln(R_1R_2R_3)^2)' = \delta(n_1R_1^2 + n_2R_2^2 + n_3R_3^2) \quad (11)$$

and may be regarded as the Hamiltonian constraint. It follows immediately that (anti-)self-dual solutions are possible for all Bianchi types of class A, including Bianchi type II! The corresponding solutions are given by

TYPE I:

$$R_i = a_i, \ i = 1,2,3; \quad (12a)$$

TYPE II:

$$R_1^2 = r^6F^{1/2}(\tfrac{1}{2}\delta r^4 + a_1)^{-1}, \ R_i^2 = r^6F^{1/2}a_i^{-1}, \ i = 2,3; \quad (12b)$$

TYPES VI_0, VII_0:

$$R_i^2 = r^6F^{1/2}(\tfrac{1}{2}\delta n_i r^4 + a_i)^{-1}, \ i = 1,2;$$
$$R_3^2 = r^6F^{1/2}a_3^{-1}; \quad (12c)$$

TYPES VIII, IX:

$$R_i^2 = r^6F^{1/2}(\tfrac{1}{2}\delta n_i r^4 + a_i)^{-1}, \ i = 1,2,3, \quad (12d)$$

where $dr = r^{-3}(R_1R_2R_3)^2\, d\eta$, $F^{1/2} = r^{-6}(R_1R_2R_3)^2$ and a_i = const. The Bianchi type IX solution with $\delta = 1$ has been first given by Belinskii *et al.*[4] (see also Gibbons ans Pope[12]). All other solutions are new. The solutions (12c) and (12d) are the first triaxial Bianchi types VI_0, VII_0, VIII, and IX solutions.

Our next task is to discuss locally rotationally symmetric (LRS) solutions of the Eguchi–Hanson[8] types EH(I) and EH(II). For the Bianchi type II space-time we take

$$EH(I){:}\ R_1 = rg, R_2 = R_3 = r, \quad (13a)$$

$$EH(II){:}\ R_1 = r, \ R_2 = R_3 = rg, \quad (13b)$$

where $dr = f^{-1}R_1R_2R_3\, d\eta$ and f,g are functions of r. We obtain from (10) the corresponding field equations which are analogous to those of the Bianchi type IX space-time considered by Eguchi and Hanson:

$$EH(I){:}\ 2g + rg' = 0, \ 2\delta = fg, \ (\ )' = d/dr; \quad (14a)$$

$$EH(II){:}\ 2g + rg' = 0, \ f = -2\delta g^2; \quad (14b)$$

with solutions

$$g = ar^{-2}, \ a = \text{const.} \quad (15)$$

Next we consider the Bianchi types VII_0 (I), VIII, and IX. We take

$$EH(I){:}\ R_1 = R_2 = rg, \ R_3 = r; \quad (16a)$$

$$EH(II){:}\ R_1 = R_2 = r, \ R_3 = rg; \quad (16b)$$

from which it follows that

$$EH(I){:} rg'(2g^2 - n_3) + 2g(g^2 - n_3) = 0,$$
$$\delta f(2g^2 - n_3) = 2g^2; \quad (17a)$$

$$EH(II){:}\ n_3 g(g'r + 2g) - 2 = 0, \ \delta n_3\, fg = 2; \quad (17b)$$

with solutions

$$EH(I){:}\ g^2 = \tfrac{1}{2}[n_3 \pm (n_3^2 + ar^{-4})^{1/2}]; \quad (18a)$$

$$EH(II){:}\ g^2 = n_3 + ar^{-4}, \ a = \text{const.} \quad (18b)$$

There are no Eguchi–Hanson type solutions for Bianchi type VI_0. The original Eguchi–Hanson[8] solution is given by $\delta = n_3 = 1$.

We now impose the (anti-)self-duality condition (7) on the Riemann tensor. We easily compute the individual components of $R^{\mu\nu}{}_{\alpha\beta}$ by the method described above. The results are

$$R^{0i}{}_{0i} = -(\dot{H}_i + H_i^2), \quad (19a)$$

$$R^{0i}{}_{kl} = -\frac{1}{2}\epsilon_{ikl}\left[\frac{n_iR_i}{R_kR_l}(H_k + H_l - 2H_i) + \left(\frac{n_kR_k}{R_iR_l} - \frac{n_lR_l}{R_iR_k}\right)(H_k - H_l)\right], \quad (19b)$$

$$R^{ik}{}_{ik} = -H_iH_k + \frac{1}{2}\epsilon_{ikl}\left(\frac{n_in_l}{R_k^2} + \frac{n_kn_l}{R_i^2} - \frac{n_in_k}{R_l^2}\right) + \frac{1}{4}\epsilon_{ikl}\left[\left(\frac{n_iR_i}{R_kR_l}\right)^2 + \left(\frac{n_kR_k}{R_iR_l}\right)^2 - 3\left(\frac{n_lR_l}{R_iR_k}\right)^2\right], \quad (19c)$$

leading to the second-order differential equations

$$(\ln R_i^2)'' = \delta\epsilon_{ikl}[n_iR_i^2(\ln R_kR_lR_i^{-2})' + (n_kR_k^2 - n_lR_l^2)(\ln R_kR_l^{-1})'] + 2(\ln R_i)'(\ln R_kR_l)'. \quad (20)$$

In addition we have

$$4[(\ln R_1)'(\ln R_2R_3)' + (\ln R_2)'(\ln R_3)'] = -[n_1^2R_1^4 + n_2^2R_2^4 + n_3^2R_3^4] + 2[n_1n_2(R_1R_2)^2 + n_1n_3(R_1R_3)^2 + n_2n_3(R_2R_3)^2], \quad (21)$$

which presents the Hamiltonian constraint. Equation (21) is a first integral of (20) and may be regarded as a constraint on the initial values of R_i and R_i' which is preserved by the evolution equations (20). Equations (20) lead, after a single integration to the equations

$$(\ln R_i^2)' = \delta\epsilon_{kli}[n_kR_k^2 + n_lR_l^2 - n_iR_i^2] - 2\lambda_iR_kR_l, \quad (22)$$

where λ_i are constants. From the constraint equation (21) it follows that the λ_i must obey

$$\lambda_i\lambda_k = \lambda_l n_l. \quad (23)$$

If $\lambda_i = 0$ Eqs. (22) reduce to Eqs. (10), obtained from the (anti-)self-duality condition (6) without any integration. If $\lambda_i \neq 0$ we obtain a richer spectrum of possible solutions. However, for the Bianchi types VIII and IX we have been unable to integrate (22) except when $R_1 = R_2$ (see also Gibbons and Pope[12]), which leads to the (anti-)self-dual Euclidean Taub–NUT metrics. The Taub–NUT–Bianchi type IX solution has been first given by Hawking[3] (see also Tseytlin[13] and Boutaleb-Joutei[14]) and the type VIII solution has been found by us very recently (Lorenz[15]). For the remaining cases we obtain the new (anti-)self-dual solutions.

TYPE I:

$$R_i = a_i, R_k = a_k, R_l = b_l \exp(-2\lambda_3 a_i a_k \eta), \quad l \neq i,k; \tag{24a}$$

TYPE II:

$$\begin{aligned} R_1^2 &= [\delta(\eta - \eta_0)]^{-1}, \\ R_2^2 &= \delta(\eta - \eta_0)\exp[-2\lambda_2 b(\eta - \eta_1)], \\ R_3^2 &= b\delta(\eta - \eta_0); \end{aligned} \tag{24b}$$

TYPE VI$_0$:

$$\begin{aligned} R_1^2 &= a\tan[-a\delta(\eta - \eta_0)], \quad R_2^2 = a^2 R_1^{-2}, \\ R_3^2 &= \sin[-2a\delta(\eta - \eta_0)]\exp[-2\lambda_3 a(\eta - \eta_1)]; \end{aligned} \tag{24c}$$

TYPE VII$_0$:

$$\begin{aligned} R_1^2 &= a\coth[-a\delta(\eta - \eta_0)], \quad R_2^2 = a^2 R_1^{-2}, \\ R_3^2 &= \sinh[2a\delta(\eta - \eta_0)]\exp[-2\lambda_3 a(\eta - \eta_1)], \end{aligned} \tag{24d}$$

where a, b, a_i, b_i, η_i are constants of integration.

IV. CONCLUSION

We have given a complete discussion of all (anti-)self-dual solutions for diagonal Bianchi types of class A. There is no difficulty in applying our method to solve the corresponding field equations in a pseudo-Riemann space-time. Besides being new exact solutions to Einstein's field equations, the solutions are double self-dual solutions of O(4) Yang–Mills equations.[16,17] The topological properties of our new solutions will be discussed in a future paper. We finally would like to point out that the complete set of (anti-)self-dual solutions for the Bianchi types of class B has been discussed by us recently.[18] In addition, the homogeneous space-times of the Kantowski–Sachs class has been considered by us very recently.[19]

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Solutions of Einstein–Yang–Mills equations with plane symmetry

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The Einstein–Yang–Mills system is solved with the assumption of plane symmetry. We present a class of abelian and a class of SO(3) nonabelian solutions of the Yang–Mills equations.

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1. INTRODUCTION

Here we present a class of abelian and a class of SO(3) nonabelian exact solutions of the system of Einstein–Yang–Mills (EYM) field equations in the absence of charge. The solutions are obtained when both the metric tensor $g_{\mu\nu}$ and the YM field tensor $F^a_{\mu\nu}$ have plane symmetry in the sense that they remain invariant under the group of motions that characterize plane symmetry.[1] In Sec. 2, we enunciate the system of EYM field equations and try to solve it in analogy to the Einstein–Maxwell (EM) problem.[2,3] We notice that the geometry of space-time is unaffected by the internal structure of the YM fields. In Sec. 3, we write the YM equations with respect to the solution of the line element. In Sec. 4, we present a class of abelian and a class of SO(3) nonabelian solutions of the YM field equations.

2. THE FIELD EQUATIONS

The EYM field equations are given by[4]

$$R_{\mu\nu} = KT_{\mu\nu} = K(-F^a_{\mu\alpha}F^a_{\mu\alpha} + \tfrac{1}{4}g_{\mu\nu}F^a_{\alpha\beta}F^{\alpha\beta}_a), \quad (1)$$

$$(\sqrt{-g}F^{\mu\nu}_a)_{,\nu} + \epsilon f_{abc}\sqrt{-g}A^b_\nu F^{\mu\nu c} = 0, \quad (2)$$

where $\mu,\nu = 0,1,2,3$; $a = 1,2,\ldots, n$ are the space-time and internal indices, respectively; n stands for the number of generators of the nonabelian gauge group, compact and semisimple. The YM fields in the equations above read

$$F^a_{\mu\nu} = A^a_{\nu,\mu} - A^a_{\mu,\nu} + \epsilon f^a_{bc}A^b_\mu A^c_\nu. \quad (3)$$

We consider that the YM fields $F^a_{\mu\nu}$ remain invariant under infinitesimal transformations like[1]

$$x'^\mu = x^\mu + \xi^\mu(x^\alpha), \quad (4)$$

which means that the Lie derivative of $F^a_{\mu\nu}$ with respect to the vector field ξ^μ vanishes,

$$\mathscr{L}_\xi F^a_{\mu\nu} = F^a_{\mu\nu,\alpha}\xi^\alpha + F^a_{\mu\lambda}\xi^\lambda_{,\nu} + F^a_{\lambda\nu}\xi^\lambda_{,\mu} = 0. \quad (5)$$

For the plane symmetric space-time, we take the line element in Taub's form,[5]

$$ds^2 = e^u dx^+ dx^- - e^v((dx^2)^2 + (dx^3)^2), \quad (6)$$

where u and v are functions of $x^\pm = x^0 \pm x^1$. For the metric given in Eq. (6), the Killing vectors read as follows:

$$\xi^\mu_{(1)} = \delta^\mu_2, \quad \xi^\mu_{(2)} = \delta^\mu_3, \quad \xi^\mu_{(3)} = x^2\delta^\mu_3 - x^3\delta^\mu_2. \quad (7)$$

Equations (5) and (7) imply that the only surviving component of $F^a_{\mu\nu}$ is

$$F^a_{+-} = F^a_{+-}(x^+, x^-). \quad (8)$$

From the integration[2] of the homogeneous equations among Eqs. (1) we obtain

$$v(t), \quad t = h(x^-) + f(x^+), \quad (9)$$

where h and f are arbitrary functions of these arguments, and

$$e^u = 2(e^{v/2})' f_+ h_-. \quad (10)$$

The remaining Einstein equations (1), together with the YM field equations (2) read

$$u_{+-} + (v'' + \tfrac{1}{2}v'^2)f_+h_- = -ke^{-u}F^2, \quad (11)$$

$$v'' + v'^2 = ke^{-2u+v/2}v'F^2, \quad (12)$$

$$(v_+ - u_+)F^a_{+-} + (F^a_{+-})_+ + \epsilon f^a_{bc}A^b_+ F^c_{+-} = 0, \quad (13)$$

$$(v_- - u_-)F^a_{+-} + (F^a_{+-})_- + \epsilon f^a_{bc}A^b_- F^c_{+-} = 0, \quad (14)$$

where the prime stands for differentiation with respect to t. Making the inner product of Eqs. (13) and (14) with F^a_{+-}, we obtain

$$(v-u)_+F^2 + \tfrac{1}{2}(F^2)_+ = 0, \quad (v-u)_-F^2 + \tfrac{1}{2}(F^2)_- = 0, \quad (15)$$

and after integration it becomes

$$F^2 = F^a_{+-}F_{+-a} = c^2e^{2(u-v)}, \quad (16)$$

where c is an integration constant.

3. THE TECHNIQUE OF SOLUTION

We observe from Eqs. (16), (11), and (12) that the YM field has the same effect on the geometry as the Maxwell field has, since these equations are the same equations solved by Letelier and Tabensky[2] (corrected by Banerjee and Chakrabarty[3]) for the EM problem. We are going to return to this point in more detail in the next section. Defining $\lambda = \exp(v/2)$, Eq. (12) after substitution into Eq. (16) yields

$$2\lambda^2\lambda' + b\lambda + 2KC^2 = 0, \quad (17)$$

where b is an integration constant. The solution of Eq. (17) is given implicitly by

$$(\lambda - 2Kc^2/b)^2 + \ln(\lambda + 2Kc^2/b) = d - bt, \quad b \neq 0, \quad (18)$$

where d is a new integration constant. The analysis of Eq. (17) and the discussion of the possible solutions, follow the same line as given in Refs. 2 and 3. Considering Eqs. (9) and (10) and defining

$$x = h(x^-) - f(x^+), \quad (19)$$

the YM field equations (2) become

$$(2\lambda'/\lambda - \lambda''/\lambda')F^a_{tx} + F^{a'}_{tx} + \epsilon f^a_{bc}A^b_t F^c_{tx} = 0, \quad (20)$$

$$f^a_{bc}A^b_x F^c_{tx} = 0. \quad (21)$$

Following the lines established by Kalb[6] and Morris,[7] we write in order to satisfy Eq. (21),

$$F^a_{tx} = A^{a'}_x + \epsilon f^a_{bc} A^b_t A^c_x = \alpha_t A^a_x, \tag{22}$$

where α_t is a function of t. Then, assuming that $A^a_x \neq 0$, Eq. (20) results in

$$(2\lambda'/\lambda - \lambda''/\lambda')\alpha_t + \alpha_t^2 + \alpha_t' = 0. \tag{23}$$

Now, we define the unit vector

$$\hat{A}^a_x = A^a_x / A_x, \quad A_x = (A^a_x A_{xa})^{1/2}, \tag{24}$$

and making the inner product of Eq. (22) by $\hat{A}^a_x$, we get

$$\alpha_t = (\ln A_x)'. \tag{25}$$

After substitution of Eq. (25) into Eq. (23), we can write

$$(2\lambda'/\lambda - \lambda''/\lambda')A'_x + A''_x = 0, \tag{26}$$

which, on integration, gives

$$A_x = \alpha + \beta/\lambda, \tag{27}$$

where α and β are integration constants. In Eq. (27), we have the modulus of the vector with components A^a_x. In order to have information about the internal directions, we need an ansatz of solution. The other vector A^a_t may be found from Eq. (21), which can be written as

$$A^a_t = (1/\epsilon)(f^a_{bc} \hat{A}^{b'}_x \hat{A}^c_x + a_t \hat{A}^a_x), \tag{28}$$

where $a_t = \epsilon \hat{A}^a_x A_{ta}$ is an arbitrary function.

4. ABELIAN SOLUTIONS

Let us look for abelian solutions of Eqs. (20) and (21). We introduce the n parameters γ^a which satisfy the constraint,[8]

$$g_{ab}\gamma^a\gamma^b = 1, \tag{29}$$

where g_{ab} is the invariant metric of the n parameters Lie group. The YM potentials and fields can be written now:

$$A^a_t = \gamma^a\varphi, \quad A^a_x = \gamma^a\psi, \quad F^a_{tx} = \gamma^a\psi', \tag{30}$$

where φ and ψ are the potentials corresponding to an EM solution in plane symmetry. If Eq. (21) is satisfied identically, then φ is an arbitrary function. Equation (20) turns into

$$(2\lambda'/\lambda - \lambda''/\lambda')\psi' + \psi'' = 0. \tag{31}$$

Integrating Eq. (31) we have, as we have analogously obtained in Eq. (27),

$$\psi = A + B/\lambda, \tag{32}$$

where A and B are integration constants. The function $\lambda(t)$ is the solution of Eq. (17). When $b \geqslant 0$ the solution is static, but when $b < 0$ it may be static or time dependent.[2,3]

5. CLASS OF SO(3) SOLUTIONS

We assume that the unit vector $\hat{A}^a_x$ has the form

$$\hat{A}^a_x = \delta^a_2 \sin\phi - \delta^a_3 \cos\phi, \tag{33}$$

where ϕ is an arbitrary function of t. Hence, by Eqs. (24), (27), and (28) we can write

$$A^a_x = (\alpha + \beta/\lambda)(\delta^a_2 \sin\phi - \delta^a_3 \cos\phi), \tag{34}$$

$$A^a_t = (1/\epsilon)[f^a_{23}\phi' + a_t(\delta^a_2 \sin\phi - \delta^a_3 \cos\phi)], \tag{35}$$

and the YM fields (22) become

$$F^a_{tx} = (\alpha + \beta/\lambda)(\delta^a_2 \sin\phi - \delta^a_3 \cos\phi). \tag{36}$$

Equations (34)–(36) give a class of nonabelian solutions due to the arbitrariness of the function $\phi(t)$. If ϕ is constant then we have a corresponding class of abelian solutions.

We observe that the solutions here obtained are not simply EM solutions, since the dependence of the YM fields on the internal directions need not be the same dependence of the charge of a test particle. This means that a nonabelian test particle feels the presence of the YM field.[8] However, the effect of the YM field on the geometry is the same as the Maxwell field, which means that the YM internal structure of the field is imperceptible to an abelian particle.

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Structure and motion of the Lee–Yang zeros

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For an Ising model satisfying the Lee–Yang condition, the zeros of the partition function Z and those of the associated functions Z_A in the space of imaginary magnetic fields at all lattice sites are determined by a single analytic hypersurface. The sense of motion of the zeros of Z as the interactions are varied can be related to the positions of the zeros of the Z_A. Contrary to a plausible conjecture, it is not true that all of the zeros of Z in a uniform field tend towards the point $\hat{z} = 1$ in the complex fugacity plane as the temperature is lowered, but it is possible that the first zero (that nearest to $\hat{z} = 1$) has a monotone motion. Various simplicity and intertwining properties of the zeros of Z and Z_A which generalize earlier results are proved by a new argument which makes direct use of the Lee–Yang property.

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I. INTRODUCTION

A new chapter in the mathematical theory of phase transitions began with the proof by Lee and Yang[1] that the zeros of the partition function Z of an Ising ferromagnet lie on the unit circle in the complex fugacity $\hat{z}$ plane. Since then there have been a number of extensions of this result to other systems, alternative proofs of the original Lee–Yang result (or modifications of it), and related studies.[2] In this paper we consider Ising magnets for which the zeros fall on the unit circle, and we ask what one can say in general (i.e., without restriction to a specific lattice or nearest-neighbor interactions, etc.) about the location of these zeros and how they move as various parameters of the system, such as the interactions, are varied.

Our discussion is limited to finite systems, but a significant motivation for studies of this sort comes from the role—again, first pointed out by Yang and Lee[3]—which zero distributions play in the infinite volume or themodynamic limit. In particular, a spontaneous magnetization can arise (or, more generally, a nonanalytic behavior of the free energy as a function of the magnetic field) if the zeros approach the point $\hat{z} = 1$ ($\zeta = 0$ in the notation used below) in the thermodynamic limit. It is thus not implausible to expect that decreasing the temperature (which means increasing interations in the notation of Sec. IV) or increasing the size of the system might shift all of the zeros towards $\hat{z} = 1$ for an arbitrary finite system (with, say, ferromagnetic pair interactions). Behavior of this type is exhibited by a linear chain with equal nearest-neighbor interactions and periodic boundary conditions.[1] Baker[4] has suggested that the same may be true for other lattices (again, with equal nearest-neighbor interactions) and has shown that this is at least consistent with some results obtained by series expansions. Fisch[5] has claimed that the zeros of the magnetization (which intertwine those of Z; see Theorem 3.6) for a system with a random distribution of ferromagnetic bonds has a similar behavior. However, we shall show by means of counterexamples (Sec. VD) that it is in general *not* true that, for an arbitrary finite Ising system with ferromagnetic pair interactions, all the zeros of the partition function (or magnetization) will move towards $\hat{z} = 1$ as the interactions increase, or the temperature is lowered, or the size of the system increases. It is still plausible that such a result might hold for a more restricted class of systems, or a less general assertion might hold for all finite systems of this type; our own (unproven) proposals are in Sec. IVC.

Following various definitions and some preliminary lemmas in Sec. II, a major part of this paper, Sec. III, is devoted to the structure of zeros in the space of independent, imaginary-valued magnetic fields at the different lattice sites. Again, the use of such independent (complex valued) fields appears in the original Lee and Yang's paper,[1] and has been fundamental to several later studies; the basic result which Lee and Yang obtained has by now become a definition,[2,6] the "Lee–Yang condition" (Sec. II). It turns out that this condition along with the appropriate spin-reversal symmetry is a natural framework for discussing the problem of zeros, and we use it in Sec. III to show that all the zeros of Z and also those of the associated function Z_A are determined entirely by a single periodic, smooth (analytic) hypersurface whose basic properties are indicated in Theorems 3.2–3.5. This result follows in a straightforward and intuitive way from the fact, pointed out in Lemma 2.4, that functions satisfying the Lee–Yang condition (in the case of an Ising model) have, under appropriate conditions, a phase which advances monotonically with the imaginary part of the magnetic field. The same procedure gives an elementary proof, Theorem 3.6, of the simplicity of the zeros of Z as a function of a single parameter, and certain intertwining properties, thus generalizing a result of Heilmann and Lieb.[7]

In Secs. IV and V we consider how the zeros move as various interactions are varied. It turns out that the sense of motion—towards or away from $\hat{z} = 1$ ($\zeta = 0$)—depends on the position of the zero relative to zeros of the quantities Z_A. This and related results will be found in Theorems 4.8–4.11,

[a] Present address.
[b] Permanent address.

and they provide a starting point for the studies of zero motion contained in Sec. V. The latter are somewhat of a disappointment in that we have only been able to prove results in rather specific cases of small systems or open structure (Cayley trees). In particular, our main conjectures of Sec. IVC remain open, although we are able to give some indication of where counterexamples are *not* to be found and also, by means of specific calculations for systems with small number of sites, Sec. VD, why certain more general conjectures will not work.

In writing the paper we have found it convenient to summarize in a number of lemmas certain results which are already in the literature (in essentially or precisely the same form), or easily derived therefrom, or of a rather elementary character. These are Lemmas 2.1–2.3, 2.6, 3.1, 4.1–4.3, 4.5, and 4.6, and for these we disclaim originality. They are included either because they help to give a more complete picture of what is known of the structure of zeros (as, for example, Lemma 4.6), or else because they are needed elsewhere (as, for example, Lemma 4.3). The most interesting of the results which we believe to be either new or significant extensions of work previously published are Lemma 2.4, Theorems 3.2, 3.3, 3.6, 4.8 (along with Corollary 4.9), 4.11, 4.12, 5.4, 5.7, 5.8, 5.11, and the examples of Sec. VD.

II. DEFINITIONS AND PRELIMINARY RESULTS

In this paper we consider a class of functions

$$Z(h) = \Sigma_\sigma f(\sigma) e^{h\cdot\sigma}, \tag{2.1}$$

where h is a vector whose n components are the complex numbers

$$h_j = \xi_j + i\eta_j, \tag{2.2}$$

σ a vector whose n components σ_j are $+1$ or -1, and $f(\sigma)$ a function with (in general) complex values. In (2.1), $h\cdot\sigma$ stands for $\Sigma_j h_j\sigma_j$ and Σ_σ for a sum over the 2^n different values of σ.

We shall use the notation $\xi = 0$, $\xi \geqslant 0$, $\xi > 0$, to indicate $\xi_j = 0$, $\xi_j \geqslant 0$, and $\xi_j > 0$, respectively, for every j, and the special notation

$$\xi > \geqslant 0 \tag{2.3}$$

to indicate $\xi \geqslant 0$ with the additional requirement that, for at least one j, ξ_j is strictly positive. Similarly, $\sigma = 1$ indicates $\sigma_j = 1$ for all j, and $-\sigma$ a vector in which $-\sigma_j$ replaces σ_j for every j. An analogous notation is employed for other vectors.

A subset A of $N = \{1,2,\ldots,n\}$ contains $|A|$ elements, and $\varnothing$ denotes the empty set. The product AB of two subsets is to be understood as the symmetric difference $(A\setminus B)\cup(B\setminus A)$. With this notation we define

$$\sigma_A = \prod_{j\in A}\sigma_j, \tag{2.4}$$

$$Z_A(h) = \Sigma_\sigma \sigma_A f(\sigma) e^{h\cdot\sigma}, \tag{2.5}$$

$$Z_A^+(h) = 2^{-|A|}\Sigma_\sigma\left(\prod_{j\in A}(1+\sigma_j)\right) f(\sigma) e^{h\cdot\sigma}. \tag{2.6}$$

Note that $Z_\varnothing$ is the same as Z, and Z_A^+ is obtained from (2.1) by omitting all terms in the sum for which $\sigma_j = -1$ for some $j\in A$. As a matter of notational convenience we shall write Z_1^+, Z_{12}, etc. in place of $Z_{\{1\}}^+$, $Z_{\{1,2\}}$, etc., and Z_{kA} where kA is the symmetric difference of $\{k\}$ and A.

Using the fact that

$$\exp i\eta_j\sigma_j = \cos\eta_j + i(\sin\eta_j)\sigma_j, \tag{2.7}$$

we can write

$$Z_A(h) = (-i)^{|A|} Z(h + (i\pi/2)\delta^A), \tag{2.8}$$

where δ^A is a vector with components δ_j^A equal to 1 when $j\in A$ and 0 otherwise. Another useful consequence of (2.7) is

$$Z_A(h + i\pi\Delta) = (-1)^{\Sigma_j\Delta_j} Z_A(h), \tag{2.9}$$

where Δ is any vector with integer components.

We define a vector z with components

$$z_j = e^{-2h_j}, \tag{2.10}$$

and a function

$$\hat{Z}(z) = Z\exp(-\Sigma_j h_j) = \Sigma_\sigma f(\sigma)\prod_j z_j^{(1-\sigma_j)/2}. \tag{2.11}$$

More generally, we shall write $\hat{Z}_A$, $\hat{Z}_A^+$, etc. for Z_A, Z_A^+, etc. multiplied by the same exponential factor as in (2.11) and expressed as functions of z. These quantities are multinomials in the components of z, with each component appearing to the zeroth or first power. Note in particular that $\hat{Z}_A^+$ is obtained from $\hat{Z}$ by setting $z_j = 0$ for every $j\in A$. For the definition which follows we use $|z| < 1$ and $|z| \leqslant 1$ to indicate $|z_j| < 1$ and $|z_j| \leqslant 1$, respectively, for all j, while $|z| < \leqslant 1$ means $|z| \leqslant 1$ and that $|z_j|$ is strictly less than 1 for at least one j.

We shall say that $\hat{Z}$, or equivalently f or Z, satisfies the *Lee–Yang condition* provided $|z| < \leqslant 1$ implies that $\hat{Z} \neq 0$. Similarly, the *weak* Lee–Yang condition is that $|z| < 1$ implies that $\hat{Z}$ is not zero, while the *strong* Lee–Yang condition is that $\hat{Z} \neq 0$ for $|z| \leqslant 1$. Equivalent conditions in terms of Z are as follows.

Lemma 2.1: Any one of the Lee–Yang conditions implies that $f(\sigma = 1) \neq 0$. Conversely, if $f(\sigma = 1) \neq 0$ and $Z \neq 0$ for $\xi > 0$ or for $\xi \geqslant 0$ or $\xi > \geqslant 0$, then the weak, the strong, and the (intermediate) Lee–Yang conditions, respectively, are satisfied.[8]

Proof: The first assertion follows from noting that $\hat{Z} = f(1)$ when $z = 0$. For the converse, consider the strong Lee–Yang condition, as the other cases can be proved by obvious modification of the following argument. From (2.11) it is evident that the nonvanishing of Z for $\xi \geqslant 0$ implies $\hat{Z} \neq 0$ for $|z| \leqslant 1$ except for the case in which one or more of the z_j is equal to zero. Let m be the minimal number of z_j which must be set equal to zero for $\hat{Z}$ to vanish, and assume that $\hat{Z} = 0$ when $z_1 = z_2 = \cdots = z_m = 0$, and $z_j \neq 0$ for $j > m$. Write $\hat{Z}$ in the form

$$\hat{Z} = a + bz_m, \tag{2.12}$$

where a and b are functions of the z_j with $j > m$ and $z_j = 0$ for $j < m$. With that choice of z_j, $j > m$, which yields the zero of $\hat{Z}$, $a = 0$, but b cannot vanish, for, if it did, we could choose a nonzero value of z_m and still have $\hat{Z} = 0$, contradicting the notion that m is the minimum number of components of z which must vanish if $\hat{Z} = 0$. Thus a zero of $\hat{Z}$ will result when

$$z_m = -a/b. \tag{2.13}$$

We can consider the right side as a function of the z_j for $j > m$ on the region

$$0 < |z_j| \leqslant 1. \tag{2.14}$$

Since a and b are continuous functions on (2.14), the only way to avoid a nonzero solution to (2.13) is for a to vanish identically on (2.14), and therefore also, by continuity, at $z_{m+1} = \cdots = z_n = 0$. But in this case $\hat{Z}$ vanishes at $z = 0$, which means $f(1) = 0$.

Lemma 2.2: If, for some $A \subset N$, Z_A satisfies the Lee–Yang condition, or the strong or weak condition, then the same condition (same strength) is satisfied by Z_B for any $B \subset N$.[9]

Proof: This result is a consequence of (2.8) and Lemma 2.1 when one notes that Z_A, (2.5), is of the form (2.1) with f replaced by

$$f_A(\sigma) = \sigma_A f(\sigma), \tag{2.15}$$

and thus $f_A(1) = f(1)$.

Lemma 2.3: If Z satisfies the Lee–Yang condition, Z_A^+ with $|A| \geqslant 1$ satisfies the strong Lee–Yang condition.

Proof: This follows from the observation that $\hat{Z}_A^+$ is obtained from $\hat{Z}$ by setting $z_j = 0$ for j in A.

If Z satisfies one of the Lee–Yang conditions, its phase $\Phi(Z)$ can be defined unambiguously on the simply connected domain where it is known not to vanish, apart from a choice of a multiple of 2π which can be made once for all (independent of h). This observation and the following lemma are fundamental for our results in Sec. III.

Lemma 2.4: If Z satisfies the Lee–Yang condition, then on the domain $\xi > \geqslant 0$ its phase Φ as a function of one component η_j of η (the other components and ξ remaining fixed) satisfies

$$\frac{\partial \Phi}{\partial \eta_j} > 0, \tag{2.16}$$

and, when η_j increases by π, Φ increases by π. If Z satisfies the strong (weak) Lee–Yang condition, the same is true on the corresponding domain $\xi \geqslant 0$ ($\xi > 0$).[10]

Proof: Assume that Z satisfies the Lee–Yang condition (the proof for the other cases is analogous). The dependence of $\hat{Z}$ on z_j is of the form

$$\hat{Z} = a + bz_j, \tag{2.17}$$

where a and b are functions of the other z_k. For $|z| \leqslant 1$, we have $|a| > 0$ and $|b| \leqslant |a|$, for otherwise we could have $\hat{Z} = 0$ with $|z_j| < 1$. Indeed, if $|z_k| < 1$ for some $k \neq j$, then $|b| < |a|$, for in that case $\hat{Z} \neq 0$ even when $|z_j| = 1$. This means that for $|z| < \leqslant 1$ it is always true that

$$|bz_j| < |a|. \tag{2.18}$$

Now the dependence of Z on η_j is of the form

$$Z = Ce^{i\eta_j} + De^{-i\eta_j}, \tag{2.19}$$

and it is easy to check that (2.18) implies that

$$|C| > |D|. \tag{2.20}$$

Then it is easy to verify that, as a function of η_j, Z in (2.19) traces out an ellipse centered at the origin in the complex plane, moving in the positive (counterclockwise) sense as η increases.

Lemma 2.5: If Z satisfies the Lee–Yang condition, then for $\xi > \geqslant 0$ the phases of Z, Z_j, and Z_j^+ are related by

$$|\Phi(Z) - \Phi(Z_j)| < \pi/2, \tag{2.21a}$$

$$|\Phi(Z) - \Phi(Z_j^+)| < \pi/2, \tag{2.21b}$$

$$|\Phi(Z_j) - \Phi(Z_j^+)| < \pi/2, \tag{2.21c}$$

where integer multiples of 2π have been added (if necessary) to the phase differences in order to minimize the terms on the left side. If Z satisfies the strong (weak) Lee–Yang condition, these inequalities hold for $\xi \geqslant 0$ ($\xi > 0$). They also hold with Z, Z_j, and Z_j^+ replaced by $\hat{Z}$, $\hat{Z}_j$, and $\hat{Z}_j^+$, respectively, on the domains $|z| \leqslant 1$, $|z| < 1$, and $|z| < \leqslant 1$ in the case where the strong, weak or (intermediate) Lee–Yang condition is satisfied.

Proof: We consider only the (intermediate) Lee–Yang condition, as the proof for the other cases is analogous. In the notation of (2.17),

$$\hat{Z}_j = a - bz_j, \quad \hat{Z}_j^+ = a, \tag{2.22}$$

and, using (2.18), it is easy to show that $\hat{Z}/\hat{Z}_j$, $\hat{Z}/\hat{Z}_j^+$, and $\hat{Z}_j/\hat{Z}_j^+$ have positive real parts. This yields (2.21) with Z, etc. replaced by $\hat{Z}$, etc. But for $|z| > 0$, $\hat{Z}$ and Z differ by the same exponential factor, (2.11), and thus by the same phase as $\hat{Z}_j$ and Z_j or $\hat{Z}_j^+$ and Z_j^+.

In Sec. IV we shall make use of the following results on functions satisfying the Lee–Yang condition.

Lemma 2.6: If $f(\sigma_1,\ldots,\sigma_n)$ and $f'(\sigma_1',\ldots,\sigma_m')$ both satisfy the Lee–Yang condition, then so does

$$f''(\sigma_1,\ldots,\sigma_m') \equiv f(\sigma_1,\ldots,\sigma_n) f'(\sigma_1',\ldots,\sigma_m'),$$

provided at least one argument of f (and possibly more) is identical with one argument of f' (i.e., f'' has at most $n + m - 1$ independent arguments).[6]

For the proof, see Refs. 6 and 12.

III. SIMPLICITY OF ZEROS AND STRUCTURE OF ZERO SURFACES

In this section we shall consider functions f satisfying

$$f(-\sigma) = f^*(\sigma), \tag{3.1}$$

i.e., changing every σ_i to $-\sigma_i$ results in changing f to its complex conjugate. In addition, we shall wish to consider cases in which f is real or f is imaginary. The following lemma summarizes some properties of Z and Z_A which follow at once from the definitions (2.1) and (2.5).

Lemma 3.1: If f satisfies (3.1), then, for $\xi = 0$, Z_A is real when $|A|$ is even (including the case $|A| = 0$ for which $Z_\varnothing = Z$) and imaginary when $|A|$ is odd. If in addition f is real for all σ, or f is imaginary for all σ,

$$Z_A(\eta) = \pm Z_A(-\eta), \tag{3.2}$$

where the $+$ sign applies in case (i) f is real and $|A|$ is even *or* f is imaginary and $|A|$ is odd—and the $-$ sign in case (ii) f is real and $|A|$ is odd *or* f is imaginary and $|A|$ is even.

We shall be interested in the zeros of Z, or more generally Z_A, as a function of the n real numbers η_j when $\xi = 0$. The main results are in Theorems 3.2–3.4.

Theorem 3.2: Suppose $\xi = 0$, and (3.1) and the Lee–Yang condition are satisfied. For A any subset of N, and k an element of N [for the notation kA, see Sec. II before (2.7)]:

(i) At some η where $Z_A(\eta) = 0$, $Z_{kA}(\eta)$ is not zero, and the sign of iZ_{kA} when $|A|$ is even, or Z_{kA} when $|A|$ is odd, is independent of k;

(ii) As a function of η_j, where j is any element of N, the other components of η held fixed, the zeros of Z_A are simple and occur at intervals of π as η_j increases;

(iii) As a function of η_j the zeros of Z_A and Z_{kA} *intertwine*: There is precisely one zero of Z_{kA} between two successive zeros of Z_A, and one zero of Z_A between two successive zeros of Z_{kA}. (Note that this intertwining implies that the sign of iZ_{kA} when $|A|$ is even, or Z_{kA} when $|A|$ is odd, alternates at successive zeros of Z_A.)

Proof: We shall consider only the case in which $A = \varnothing$, so $Z = Z_A$. [The case of general A reduces to this upon observing when Z satisfies the Lee–Yang condition, so does Z_A, and when $|A|$ is even, $f_A(\sigma)$, (2.15), satisfies (3.1) along with $f(\sigma)$. When $|A|$ is odd, one considers iZ_A, and again the counterpart of (3.1) is satisfied.] Note that

$$Z_k^+ = \tfrac{1}{2}(Z + Z_k) \tag{3.3}$$

satisfies the strong Lee–Yang condition, Lemma 2.3, and thus it does not vanish when $\xi = 0$. Its phase satisfies (2.16) and advances by π every time η_j increases by π. But since Z is real and Z_k is pure imaginary, Lemma 3.1, the zeros of Z occur when the phase of Z_k^+ is an odd multiple of $\pi/2$, and those of Z_k when the phase is an even multiple of $\pi/2$. These observations establish (i), (ii), and (iii) aside from the second assertion in (i). To establish that, we consider some l in N unequal to k. In Lemma 2.5, replace Z by Z_k^+, j by l, and Z_j^+ by Z_{kl}^+. Since Z_k^+ satisfies the strong Lee–Yang condition, the counterpart of (2.21b),

$$|\Phi(Z_k^+) - \Phi(Z_{kl}^+)| < \pi/2, \tag{3.4}$$

applies when $\xi = 0$. Combining this with the corresponding inequality with k and l interchanged shows that the phases of Z_k^+ and Z_l^+ differ (mod 2π) by *less* than π, whereas if iZ_k and iZ_l had opposite signs at a zero of Z, the phase difference would have to be *exactly* π.

The zeros of Z lie on an infinite set of smooth hypersurfaces in the space $\mathbb{R}^n$ spanned by the components of η. As these surfaces are obtained from each other by appropriate translations, a knowledge of just one of them determines them all, and indeed all the $Z_A = 0$ surfaces for every $A \subset N$. The situation is summarized in the following theorem where, for convenience, the surfaces are represented by letting η_n be a function of

$$\tilde{\eta} = (\eta_1, \eta_2, \ldots, \eta_{n-1}). \tag{3.5}$$

We also use the notation $\tilde{A}$ for $A \setminus \{n\}$; and define $\epsilon(A,B)$ to be 1 if $n \notin A$ and $n \in B$, -1 if $n \in A$ and $n \notin B$, and 0 otherwise.

Theorem 3.3: When the Lee–Yang condition and (3.1) are satisfied, and $\xi = 0$, the equation $Z_A = 0$ for $A \subset N$ results in an infinite set of surfaces, each of which has the form

$$\eta_n = F_A(\tilde{\eta}). \tag{3.6}$$

Here F_A is a real analytic function defined everywhere on $\mathbb{R}^{n-1}$ satisfying

$$\frac{\partial F_A}{\partial \eta_j} < 0, \tag{3.7}$$

$$F_A(\tilde{\eta} + \pi\delta^j) = F_A(\tilde{\eta}) - \pi, \tag{3.8}$$

for $j = 1, 2, \ldots, n-1$. By adding an integer multiple of π to $F_A(\tilde{\eta})$, one obtains a function $\hat{F}_A(\tilde{\eta})$ describing another $Z_A = 0$ surface, and all such surfaces are obtained in this way. If B is another subset of N, then

$$\eta_n = F_B(\tilde{\eta}) = F_A(\tilde{\eta} + (\pi/2)[\delta^{\tilde{B}} - \delta^{\tilde{A}}]) - (\pi/2)\epsilon(A,B) \tag{3.9}$$

is a surface where $Z_B = 0$. [See the preceding paragraph for notation; the symbol δ is defined just after (2.8).]

Proof: As in Theorem 3.2, we consider the case $A = \varnothing$, that is, the surfaces of $Z = 0$. Since Z_k^+ does not vanish for $\xi = 0$, its phase Φ is well defined (once a choice has been made at $\eta = 0$) and a real analytic function of η throughout $\mathbb{R}^n$. The $Z = 0$ surfaces correspond to setting Φ equal to an odd integer times $\pi/2$. Since Φ is monotone-increasing in η_n and increases by π every time η_n is increased by π (Lemma 2.4), for every η there is precisely one value of η_n for which Φ has a specified value, and the values of η_n at which $Z = 0$ occur at intervals of π (Theorem 3.2). The analyticity of $F_\varnothing$ is a consequence of the implicit function theorem and $\partial\Phi/\partial\eta_n > 0$, while (3.7) is a consequence of (2.16).

To establish (3.8), we note that if $Z = 0$ for some η it will also (Theorem 3.2) be zero if η_j ($j < n$) is increased by π and η_n is decreased by π. What (3.8) asserts is that these two zeros are on the same $Z = 0$ surface. To see this, write, making use of (3.1),

$$\begin{aligned} Z &= ae^{i(\eta_j + \eta_n)} + a^* e^{-i(\eta_j + \eta_n)} \\ &\quad + be^{i(\eta_j - \eta_n)} + b^* e^{-i(\eta_j - \eta_n)} \\ &= 2|a|\cos(\eta_j + \eta_n + \psi) + 2|b|\cos(\eta_j - \eta_n + \chi), \end{aligned} \tag{3.10}$$

where a, b, ψ, and χ depend on the other components of η. By writing $\hat{Z}$ as a function of z_j and z_n, setting $z_n = 0$, and noting that the resulting function $(\hat{Z}_n^+)$ of z_j cannot vanish for $|z_j| \leqslant 1$, one can show that $|a| > |b|$. This means that if we start at a zero of Z and then increase η_j continuously, keeping $Z = 0$, the argument of the first cosine in (3.10) can never reach 0 or π, but must remain in a range where the cosine is strictly monotone with a nonvanishing derivative. Hence $\eta_j + \eta_n$ is a well-defined periodic function of $\eta_j - \eta_n$, and the value of η_n when η_j has increased by π must be its original value minus π.

Finally, one can use (2.8) and (2.9) to show that the arguments presented above for $A = \varnothing$ extend to a general $A \subset N$, and that if Z_A has a zero at η, Z_B has a zero at $\eta + (\pi/2)(\delta^A - \delta^B)$. The latter leads to (3.9).

Theorem 3.4: If in addition to satisfying the conditions of Theorem 3.3, f is real for all σ or imaginary for all σ, the functions F_A have the additional symmetry

$$F_A(\tilde{\eta}) + F_A(-\tilde{\eta}) = m\pi, \tag{3.11}$$

where m is an odd integer for case (i) of lemma 3.1 and an even integer for case (ii), and Z_A is zero at all points η of the form

$$\eta_j = (\pi/2)\Delta_j, \tag{3.12}$$

where the Δ_j are integers whose sum is odd in case (i) and even in case (ii) of Lemma 3.1. The same $Z_A = 0$ surface passes through all points (3.12) having a given $\Sigma_j \Delta_j$.

Proof: We begin the proof with case (ii), that is (3.2) holds with a minus sign. This means $Z_A = 0$ at $\eta = 0$, and if Z_A is zero at η, it is also zero at $-\eta$. Thus the surface passing through $\eta = 0$ satisfies (3.11) with $m = 0$ when $\tilde{\eta}$ is small. As the left side of (3.11) is an analytic function, the result holds everywhere. The other $Z_A = 0$ surfaces are obtained, Theorem 3.3, by adding integer multiples of π to F_A, and thus (3.11) will be satisfied with m even. Case (i) can be related to case (ii), for a given f, using (3.8) and (3.9). To establish that $Z_A = 0$ for (3.12), note that η and $-\eta$ differ by a vector $\pi\Delta$, and use (2.9) together with (3.2). That the same zero surface passes through all points with a given $\Sigma_j \Delta_j$ is a consequence of (3.8).

One is often interested in the zeros of Z (or Z_A) when the η_j depend linearly on a real parameter ζ,

$$\eta_j = g_j \zeta, \tag{3.13}$$

the g_j being real numbers. We shall study the case $g > \geqslant 0$. If $Z^{(m)}$ is the mth derivative of Z with respect to ζ, it can be written in the form

$$Z^{(m)} = \Sigma_\sigma f^{(m)}(\sigma) e^{h\cdot\sigma}, \tag{3.14}$$

where (3.14) serves to define $f^{(m)}(\sigma)$. Similarly the mth derivative of Z_A, $Z_A^{(m)}$, can be written in the form (3.14) with $f^{(m)}$ replaced by

$$f_A^{(m)}(\sigma) = \sigma_A f^{(m)}(\sigma); \tag{3.15}$$

see (2.15).

Lemma 3.5: If f satisfies (3.1), so does $f^{(m)}$. For $g > \geqslant 0$, if Z satisfies the Lee–Yang condition, then so does $Z_A^{(m)}$.

Proof: Note that

$$Z^{(1)} = i\Sigma_j g_j Z_j, \tag{3.16}$$

and that if Z satisfies the Lee–Yang condition, so do the Z_j (Lemma 2.2). Thus for $\xi > \geqslant 0$, the right side of (3.16) is a sum of terms, not all of which vanish, and whose phases are constrained relative to that of Z by (2.21a). Hence $Z^{(1)}$ cannot vanish. It is easy to see that $f(1) \neq 0$ implies $f^{(1)}(1) \neq 0$, and thus $Z^{(1)}$ satisfies the Lee–Yang condition (Lemma 2.1). It is also easy to show that $f^{(1)}$ satisfies (3.1) if f does. The results for general m follow by induction; those for general A from (3.15)—see (2.15) and (2.8).

Theorem 3.6: Assume that (3.1) and the Lee–Yang condition are satisfied, $\xi = 0$, and (3.13) holds with $g > \geqslant 0$. It is then the case that:

(i) The zeros of $Z_A(\zeta)$ and $Z_{kA}(\zeta)$ are simple and intertwine (as defined in Theorem 3.2).[13]

(ii) The zeros of $Z_A^{(m)}(\zeta)$ are simple.

(iii) The zeros of $Z_A(\zeta)$ intertwine those of $Z_A^{(1)}(\zeta)$, and for $m \geqslant 1$ the zeros of $Z_A^{(m)}(\zeta)$ intertwine those of $Z_A^{(m+1)}(\zeta)$.

Proof: We can, as usual, restrict the proof to $A = \varnothing$. Let Φ be the phase of Z_k^+. Then Lemma 2.4 along with $g > \geqslant 0$ implies that $d\Phi / d\zeta > 0$, from which (i) follows precisely as in the proof of Theorem 3.2. To prove (ii) and (iii), we define

$$Z^+ = Z - iZ^{(1)} = Z + \Sigma_j g_j Z_j. \tag{3.17}$$

The argument employed in Lemma 3.5 shows that Z^+ does not vanish for $\xi > \geqslant 0$, and it is easy to show that the corresponding $f^+(1)$ does not vanish. On the other hand, Z^+ also does not vanish when $\xi = 0$, because Z is real, the Z_j are pure imaginary (Lemma 3.1), and when $Z = 0$, $iZ_j \neq 0$ and has a sign independent of j [Theorem 3.2(i)]. Hence Z^+ satisfies the strong Lee–Yang condition, and its phase Φ satisfies $d\Phi / d\zeta > 0$. We conclude, once again following the argument of Theorem 3.2, that since Z and $Z^{(1)}$ are both real, their zeros must intertwine. Lemma 3.5 implies that the argument above could just as well be applied to $Z^{(m)}$ in the place of Z, showing that its zeros intertwine those of $Z^{(m+1)}$.

Theorem 3.7: With the conditions of Theorem 3.6 satisfied,

(i) each zero of $Z_A(\zeta)$ [or of $Z_A^{(m)}(\zeta)$] is a real analytic function of g on the region $g > \geqslant 0$;

(ii) this function $\zeta(g)$ is everywhere strictly positive, or everywhere strictly negative, or identically equal to zero;

(iii) if $\zeta(g) > 0$, then $\partial\zeta / \partial g_j < 0$ (3.18)

for every j, whereas the reverse inequality holds for $\zeta(g) < 0$.[14]

Proof: As in the proof of Theorem 3.3, a particular zero corresponds to a particular value for a phase Φ with properties given by Lemma 2.4, in particular (2.16). Since this phase is strictly monotone increasing in ζ (see the argument of Theorem 3.6), and tends to $\pm\infty$ as ζ tends to $\pm\infty$, the function $\zeta(g)$ corresponding to this value of Φ is uniquely defined for all $g > \geqslant 0$. In the differential equation

$$d\Phi = 0 = \Sigma_j \frac{\partial\Phi}{\partial\eta_j}(\zeta\, dg_j + g_j\, d\zeta) \tag{3.19}$$

the coefficient of $d\zeta$ is never zero, so the implicit function theorem implies that $\zeta(g)$ is real analytic. To establish (ii), note that if $\zeta = 0$ is a zero of Z_A for some $g \neq 0$, then Z_A is zero at $\eta = 0$, and thus $\zeta = 0$ is a zero for all $g \neq 0$, in particular for all $g > \geqslant 0$. Finally, (3.18) is an obvious consequence of (3.19) and the fact that the $\partial\Phi / \partial\eta_j$ are all positive.

IV. MOTION OF ZEROS: GENERAL CONDITIONS

A. Introduction

Here and in Sec. V we shall assume that

$$f(\sigma) = \exp\left[\sum_{A \subset N} J_A(\sigma_A - 1)\right], \tag{4.1}$$

where σ_A is given by (2.4) and the interactions, denoted collectively by J, are noninfinite real numbers *with* $J_A = 0$ *when* $|A|$ *is odd*. It is at once evident that f is real and satisfies (3.1). We shall speak of the different values of $j = 1,2,\dots,n$ as "sites," and shall say that two of them, j and j', are *connected* by J provided there is a sequence $j = k_1, k_2, \dots, k_m = j'$ such that k_l and k_{l+1} both belong to some A with $J_A \neq 0$. If each site is connected to every other site, we shall say that the interactions are connected, or that the sites comprise a single connected component. If this is not the case, the sites will consist of two or more connected components, and f, and likewise Z, will be a product of factors corresponding to the different components.

When $|A| = 2$, we shall call J_A a "pair interaction", and will use "pair interactions" to refer to the situation in which $J_A = 0$ for $|A| \neq 2$. The interactions are "ferromagnetic" if $J_A \geqslant 0$ for all A. We shall say that J satisfies the Lee–Yang condition if the corresponding f (that is to say, the corresponding $\hat{Z}$) satisfies the Lee–Yang condition.

Lemma 4.1: Suppose that for interactions J, the set of sites consists of two or more connected components, each of which satisfies the Lee–Yang condition, and J' is obtained from J by making some pair interactions positive which were initially zero in such a manner that J' is connected. Then J' satisfies the Lee–Yang condition.

Lemma 4.2: A connected set of ferromagnetic pair interactions satisfy the Lee–Yang condition.

Lemma 4.3: If J satisfies the Lee–Yang condition and J' is obtained from J by increasing (making more positive or less negative) any J_A with $|A|=2$, then J' satisfies the Lee–Yang condition.

Proof of Lemmas 4.1, 4.2, and 4.3: All these lemmas are elementary consequences of Asano's result, Lemma 2.6. By direct calculation,

$$f_0(\sigma_1,\sigma_2) = \exp J(\sigma_1\sigma_2 - 1) \tag{4.2}$$

satisfies the Lee–Yang condition for $J>0$. If $f(\sigma_1,\sigma_2,...,\sigma_n)$ satisfies the Lee–Yang condition, then so does $f_0(\sigma_1,\sigma_2)\times f(\sigma_1,...,\sigma_n)$ or $f_0(\sigma_n,\sigma_{n+1})\times f(\sigma_1,...,\sigma_n)$. The former establishes Lemma 4.3, the latter, by iteration, Lemma 4.2. Similarly, if $f(\sigma_1,...,\sigma_n)$ and $f'(\sigma_1',...,\sigma_m')$ satisfy the Lee–Yang condition, so does

$$f_0(\sigma_1,\sigma_1')f(\sigma_1,...,\sigma_n)f'(\sigma_1',...,\sigma_m'),$$

by two applications of Lemma 2.6.

We shall be interested in the zeros of $Z_A(\zeta)$, $A\subset N$, under the condition $\xi=0$ with η given in (3.13). Some elementary but useful results are summarized in:

Lemma 4.4: Let f be given by (4.1). Then

(i) $$Z_A(\zeta) = (-1)^{|A|}Z_A(-\zeta) \tag{4.3}$$

and in particular $Z_A(0)$ vanishes if $|A|$ is odd;

(ii) if in addition the Lee–Yang condition is satisfied, then $Z_A(0)>0$ for $|A|$ even.

Proof: Assertion (i) is a consequence of Lemma 3.1. As for (ii), we note that $Z_A(0)$, i.e., at $\eta=0$, cannot vanish for even $|A|$ in light of Theorem 3.2(i), as we already know that it vanishes for all $|A|$ odd. The question of sign can be settled by continuity, noting that if all the J_B with $|B|=2$ tend to $+\infty$, $Z_A(0)=2$.

B. The case $g=1$

When $g=1$, i.e., $\eta_j=\zeta$ for all j, (2.9) implies that

$$Z_A(\zeta+\pi) = (-1)^n Z_A(\zeta). \tag{4.4}$$

Combining this with (4.3), we see that $Z_A(\zeta)$ (and hence its zeros) is completely determined by its values for

$$0\leqslant\zeta\leqslant\pi/2, \tag{4.5}$$

which we shall refer to as the *principal interval* and which corresponds to the lower half of the unit circle for the variable

$$\hat{z} = e^{-2i\zeta}; \tag{4.6}$$

see (2.10).

Lemma 4.5: Let f be given by (4.1), and assume $\xi=0$ and $g=1$. Then:

(i) the zeros of $Z_{N\setminus A}$ in the principal interval are obtained from those of Z_A by replacing ζ by $\pi/2-\zeta$;

(ii) $Z(\zeta)>0$ for $|\zeta|\leqslant\pi/2n$.

Proof: Note that these results hold whether or not the Lee–Yang condition is satisfied. The first is a consequence of the fact that, see (2.8) and (2.9), adding $\pi/2$ to every η_i carries one from a zero of Z_A to one of $Z_{N\setminus A}$. This combined with (4.3) and (4.4) leads to the desired result. The second is proved by noting that if the terms in (2.1) corresponding to σ and $-\sigma$ are combined, one can express (2.1) as a sum of cosines with strictly positive coefficients and arguments which lie between 0 and $n\zeta$. The condition on ζ in the lemma ensures that all these cosines are positive except for one which may be zero. [If some of the J_A in (4.1) are allowed to be infinite, $\zeta=\pm\pi/2n$ may be a zero of Z, though Z is still positive for $|\zeta|<\pi/2n$.]

Lemma 4.6: Assume f is given by (4.1) and satisfies the Lee–Yang condition, and $g=1$. Then:

(i) $Z_B(0)=0$ for $|B|$ odd, $Z_B(0)>0$ for $|B|$ even;

(ii) for *n even*, Z_B for even $|B|$ has $n/2$ zeros in the interior of the principal interval, and is not zero at $\zeta=\pi/2$, while when $|B|$ is odd, Z_B has $n/2-1$ zeros in the interior of the principal interval and is zero at $\zeta=\pi/2$;

(iii) for n odd, Z_B has $(n-1)/2$ zeros in the interior of the principal interval, with $\zeta=\pi/2$ a zero when $|B|$ is even but not when $|B|$ is odd.

Proof: Here (i) merely restates Lemma 4.4. The proof of (ii) and (iii) consists in noting that $\hat{Z}$ is a polynomial of degree n in the variable $\hat{z}$, (4.6), whose simple zeros, Theorem 3.6, fall on the unit circle in complex conjugate pairs or at $\hat{z}=+1$ or -1, corresponding to $\zeta=0$ or $\pi/2$. Whether there are zeros at $\hat{z}=\pm1$ can be determined with the help of (4.3) and (4.4).

C. Conjectures on the motion of zeros of $Z(\zeta)$

In view of the original discussion of Lee and Yang,[1] it is not implausible to suppose that, for $g=1$ and ferromagnetic pair interactions, the zeros in the principal interval have a tendency to move towards $\zeta=0$ as the J_A increase and towards $\pi/2$ as the J_A decrease. Indeed, it is not hard to show that all the zeros accumulate at $\pi/2$ when all the J_A go to zero. In the case of nearest-neighbor pair interactions on a closed ring, all nonzero J_A being equal, an explicit calculation shows this monotone motion.[1] However, the plausible conjecture that, for connected ferromagnetic pair interactions, *each* zero in the principal interval decreases (moves towards $\zeta=0$) as *each* J_A, $|A|=2$, increases turns out to be *false*; see Sec. VD. There are at least two weaker conjectures which seem to us to be plausible, but for which we do not have proofs (nor, needless to say, counterexamples):

Conjecture 1: For connected ferromagnetic pair interactions and for $g>\geqslant 0$, the smallest positive zero of $Z(\zeta)$ (which we call the "first zero") is a nonincreasing function of each pair interaction J_A, $|A|=2$.

Conjecture 1': Replace $g>\geqslant 0$ by $g=1$ in the condition of Conjecture 1.

Conjecture 2: In the case of ferromagnetic pair interactions with $J_A=J>0$ for *all* $|A|=2$, and $g=1$, all zeros of $Z(\zeta)$ in the interior of the principal interval are decreasing functions of J.

We shall show, Theorem 4.12, that although Conjecture 1′ seems weaker than Conjecture 1, it is in fact equivalent. Obviously, Conjecture 2 represents only one of several cases in which there is a large amount of symmetry and one might hope for stronger results than in Conjecture 1.

D. Motion of zeros

Let ζ be a simple zero of $Z_A(\zeta)$ considered as a function of J_B. By means of (4.1), and noting that $Z_A = 0$, we see that

$$\frac{d\zeta}{dJ_B} = -\frac{\partial Z_A/\partial J_B}{\partial Z_A/\partial \zeta} = -\frac{Z_{BA}}{Z_A^{(1)}}, \tag{4.7}$$

where $Z_A^{(1)}$ is the derivative of Z_A with respect to ζ in the notation of Sec. III, and BA is the symmetric difference (Sec. II). In addition to (4.7) we need the result:

Lemma 4.7: If for some ζ, both Z_A and Z_{BA} vanish, with J_B noninfinite, then both Z_A and Z_{BA} remain equal to zero at this value of ζ for *all* values of J_B, the other interactions remaining fixed.

Proof: This result follows from noting that the dependence of Z_A and Z_{BA} on J_B is of the form

$$Z_A = C + De^{-2J_B}, \qquad Z_{BA} = C - De^{-2J_B}, \tag{4.8}$$

with C and D functions of ζ and the other interactions. If Z_A and Z_{BA} vanish simultaneously, then $C = D = 0$.

Theorem 4.8: A particular simple zero of $Z_A(\zeta)$ regarded as a function of J_B, the other interactions held fixed, can behave in only one of three possible ways in any connected interval of J_B values for which the zero remains simple: (i) ζ is independent of J_B; (ii) $d\zeta/dJ_B > 0$; (iii) $d\zeta/dJ_B < 0$.

Proof: The proof consists of noting that $d\zeta/dJ_B$ is a continuous (analytic) function of J_B as long as the zero is simple, and, if it is ever equal to zero, (4.7) implies that $Z_{BA} = 0$, so that by Lemma 4.7 case (i) holds throughout the interval in question.

As a particular case, Lemma 4.2 together with Theorem 3.6 yield

Corollary 4.9: The three exclusive possibilities of Theorem 4.8 apply in particular to the interval $0 < J_B < \infty$ (or $0 \leqslant J_B < \infty$ if $J_B = 0$ leaves the interactions connected) in the case of connected ferromagnetic pair interactions and $g > \geqslant 1$.

Note that even in the case of connected ferromagnetic pair interactions, which of the three situations actually occurs will in general depend on the values of the *other* interactions; these can very well (as shown explicitly in Sec. V) change the motion from category (ii) to category (iii)—with, of course, (i) occurring at the boundary.

The category can be related to the signs of the terms on the right side of (4.7), and the following are some results which are useful in connection with Conjectures 1 and 2.

Theorem 4.10: With the Lee–Yang condition satisfied and $g > \geqslant 0$, the first (i.e., smallest positive) zero of $Z_A(\zeta)$ for $|A|$ even is a strictly increasing, strictly decreasing, or constant function of J_B depending on whether Z_{BA} is positive, negative, or zero, respectively, at this value of ζ. In particular, the first zero of $Z(\zeta)$ increases with J_B for $Z_B > 0$ and decreases for $Z_B < 0$.

Proof: Since $Z_A(0)$ is positive, Lemma 4.4, $Z_A^{(1)}$ will necessarily be negative at the first (simple—see Theorem 3.6) zero of $Z_A(\zeta)$, so that the conclusion follows from (4.7); see also Lemma 4.7 and Theorem 4.8.

Theorem 4.11: With $g > \geqslant 1$ and the Lee–Yang conditon satisfied, the pth positive zero of $Z(\zeta)$ will decrease, increase, or remain fixed as a function of J_B, $|B| = 2$, depending on whether it is larger than, smaller than, or coincides with, respectively, the pth zero of Z_B.

Proof: Suppose that $B = \{k,l\}$. Then, by Theorem 3.6, the zeros of Z intertwine the zeros of Z_k, which, in turn, intertwine the zeros of Z_{kl}. Thus between any two consecutive zeros of Z_k there will be precisely one zero of Z and one of Z_{kl}, with the pth zero of Z occuring in the same interval as the pth zero of Z_{kl}. As the signs of $Z^{(1)}$ and $Z_{kl}^{(1)}$ alternate at successive zeros [see Theorem 3.6 (iii)], and as both Z and Z_{kl} are positive at $\zeta = 0$, Lemma 4.4, the sign of $Z^{(1)}$ at the pth zero of Z is the same as that of $Z_{kl}^{(1)}$ at the pth zero of Z_{kl}. These observations can be used to determine the sign of the right side of (4.7), with $A = \varnothing$, in terms of the relative order of the pth zeros.

(In the more general case of $|B| \geqslant 4$, the motion of the pth zero of Z as a function of J_B—assuming the Lee–Yang condition satisfied—can be related to the number of zeros of Z_B which are smaller than this zero. These are obvious generalizations of this theorem with Z replaced by a more general Z_A.)

Using Theorem 4.11, one can reformulate the consequences of Conjectures 1 and 2 in the equivalent forms:

1. *The first zero of Z_A for every $|A| = 2$ either precedes or coincides with the first zero of Z.*

2. *For each A with $|A| = 2$, the zeros of Z and Z_A intertwine on the principal interval, with the first zero of Z_A preceding the first zero of Z.*

E. Equivalence of Conjectures 1 and 1′

Theorem 4.12: Conjectures 1 and 1′ are either both true or both false.

Proof: Since 1′ is a special case of 1, it will suffice to show that the falsity of 1 implies that of 1′. If 1 is false, there is some n, some $g > \geqslant 0$, and some A, $|A| = 2$, such that Z_A is positive at the first zero of Z, Theorem 4.10. By continuity, the same will be true for some g for which the g_j are strictly positive rational numbers or, equivalently, positive integers, since multiplying all the g_j by a common factor and dividing ζ by the same factor gives the same result. Consider a particular site k where g_k is larger than 1. Change g_k to 1, but add a set of $g_k - 1$ "dummy" sites $k' = 1,2,\ldots,g_k - 1$ to the system. At each of these sites, $g_{k'} = 1$, and in addition there are "dummy" pair interactions $J_{kk'} > 0$ connecting the spins at dummy sites to the spin at site k. (There are no additional interactions involving the dummy sites.) In the limit when all the $J_{kk'}$ are $+\infty$, the result is the same as it was before g_k was reduced to 1. A similar construction can be carried out at each site j where g_j exceeds 1. Continuity can again be invoked to show that when all the added dummy interactions are finite but sufficiently large, Z_A will still be positive at the first zero of Z, yielding a counterexample to 1′.

V. MOTION OF ZEROS: PARTICULAR RESULTS

In this section we present a number of results regarding the motion of zeros for rather special classes of systems. We assume throughout that $\xi = 0$, that η is related to ζ through (3.13), and that f is of the form (4.1). We shall consider the positive zeros of $Z(\zeta)$—or sometimes $Z_B(\zeta)$—with the first zero the smallest of these, the second the next smallest, etc. We find some support for Conjecture 1 (Sec. VA) and 1′ (Sec. VB), an indication of how the zeros depend on system size in a special case (Sec. VC), and counterexamples, using small systems, to some possible generalizations of these results (Sec. VD).

A. The case $g > \geqslant 0$

Theorem 5.1: Assume that $g > \geqslant 0$, and that for $J_{12} = 0$ the sites form two connected components (Sec. IV), with site 1 in one component and site 2 in the other, and each component satisfies the Lee–Yang condition. Then for $J_{12} \geqslant 0$ the first zero of $Z(\zeta)$ is a strictly decreasing function of J_{12} except in the case where $g_j = 0$ for all sites in one of the two original ($J_{12} = 0$) connected components, in which case it is independent of J_{12}.

Proof: Assume that there is some $g_j > 0$ in each component. With $J_{12} = 0$ one has

$$Z = Z^1 Z^2, \quad Z_{12} = Z_1^1 Z_2^2, \tag{5.1}$$

with Z^j the function Z calculated for component j, and the first zero of Z will occur at the fist zero of $Z^1(\zeta)$ or $Z^2(\zeta)$, whichever is smaller. For this value of ζ, both Z_1^1 and Z_2^2 will be i times a positive number [see the proof of Theorem 3.6(i) and note that Z^1 and Z^2 are positive at $\zeta = 0$], and thus Z_{12} will be negative. As the zeros of Z^1 and Z^2 are simple, Theorem 3.6, the first zero of Z will be simple when $J_{12} = 0$ provided the first zeros of Z^1 and Z^2 do not coincide. The desired result then follows from (4.7) along with Theorem 4.8 (note Lemma 4.1 and Theorem 4.10). If the first zeros of Z^1 and Z^2 coincide, Z is a minimum at its first (nonsimple) zero, but as Z_{12} is negative, a small positive J_{12} will make this minimum negative and the smaller of the two resulting zeros will continue to decrease as J_{12} increases, Theorem 4.8. Finally, assume that all the g_j are zero in one component, say the first one. Then Z_1^1 and hence Z_{12} vanishes when $J_{12} = 0$. Lemma 4.7 then shows that every zero of Z is independent of J_{12}. (The proof of Theorem 5.9 indicates an alternative route to the same conclusion.)

Although this result is far from establishing Conjecture *1*, it nonetheless has an interesting consequence:

Corollary 5.2: For $g > \geqslant 0$, consider a system with connected ferromagnetic pair interactions in which the only nonzero J_{jk} (regarded as lines connecting sites j and k) form the bonds of a Cayley tree, i.e., a graph in which there are no closed loops. Then the first zero of $Z(\zeta)$ is a nonincreasing function of each of the *nonzero* (and thus positive) J_{jk}.

It is worth emphasizing that the next result is not limited to pair interactions (though we always assume, Sec. IVA, that $J_A = 0$ if $|A|$ is odd) nor does it require that the Lee–Yang condition be satisfied.

Theorem 5.3: For $g > \geqslant 0$ and *at most three* of the g_j positive, the first zero, the smallest zero, of $Z(\zeta)$ is a monotone nonincreasing function of every J_A provided the interactions are ferromagnetic ($J_B \geqslant 0$).

Proof: We assume $g_j = 0$ for $j \geqslant 4$ and use (2.7) to write Z in the form

$$Z = \left(\prod_{j=1}^{3} \cos \eta_j\right) Z^0 \times (1 - t_1 t_2 \langle\sigma_1\sigma_2\rangle - t_2 t_3 \langle\sigma_2\sigma_3\rangle - t_1 t_3 \langle\sigma_1\sigma_3\rangle) \tag{5.2}$$

with

$$t_j = \tan \eta_j, \tag{5.3}$$

$$\langle\sigma_j\sigma_k\rangle = Z_{jk}^0 / Z^0, \tag{5.4}$$

and Z_A^0 stands for Z_A when $h = 0$. The GKS inequalities imply that the $\langle\sigma_j\sigma_k\rangle$ are nonnegative, and nondecreasing functions of each of the J_A. Thus from (5.2) it is evident that the first zero of Z occurs when the η_j are between 0 and $\pi/2$, and that at this value of ζ any increase in J_A will make Z negative or leave $Z = 0$, so that the first zero of $Z(\zeta)$ cannot increase.

Theorem 5.4: For $g > \geqslant 0$ and $n \leqslant 4$, the first zero of Z is a nonincreasing function of J_A for $|A| = 2$, in the case of connected ferromagnetic pair interactions.

Note that this implies that counterexamples to Conjecture 1 require at least $n = 5$ sites. The proof is obtained by noting that a violation of the expected monotonicity, if it occurred for $n = 4$, would also occur with one of the g_j set equal to zero, in accordance with the following lemma. But then at most three g_j would be positive, a situation covered by Theorem 5.3.

Lemma 5.5: With $g > \geqslant 0$ and f given by (4.1) satisfying the Lee–Yang condition, if Z_{12} is positive at the first zero of $Z(\zeta)$, this will also be true for some choice of $g > \geqslant 0$ with either $g_1 = 0$ or $g_2 = 0$.

Proof: Let X be the assertion that Z_{12} is positive at the first zero of $Z(\zeta)$. Then X is equivalent to the assertion that $Z - Z_{12}$ is negative at the first zero of $Z + Z_{12}$. To see this, note that both Z and Z_{12} are positive at $\zeta = 0$ (Lemma 4.4), negative at the first positive zero of Z_1, and each possesses precisely one zero in this interval, by the intertwining property of Theorem 3.6(i); see also the proof of Theorem 4.11. Hence the first zero of $Z + Z_{12}$ occurs between the first zero of Z and the first zero of Z_{12}, and Z_{12} is positive at this point if and only if it is positive at the first zero of Z.

Note next that the first zero of $Z + Z_{12}$, by the argument of Theorem 3.2, occurs when the phase of

$$Z_{12}^{+} = \tfrac{1}{4}(Z + Z_1 + Z_2 + Z_{12}) = a e^{i(\eta_1 + \eta_2)} \tag{5.5}$$

(where the right side indicates the dependence on η_1 and η_2) reaches $\pi/2$ for the first time—note that Lemmas 2.3 and 2.4 apply. Hence X is equivalent to the assertion that when this occurs,

$$Z_{12}^{-} = \tfrac{1}{4}(Z + Z_1 - Z_2 - Z_{12}) = b e^{i(\eta_1 - \eta_2)} \tag{5.6}$$

will have a negative real part, that is, a phase between $\pi/2$ and $3\pi/2$ (mod 2π). Consider η_1 and η_2 as nonnegative, adjustable parameters, and note that the phase of a increases monotonically with any $\eta_j, j\geqslant 3$. Then X is true for some choice of η_1,η_2 nonnegative if and only if for some nonnegative choice of the remaining η_j, the phase $\Phi(a)$ has not reached $\pi/2$ for the first time, while that of b is outside (mod 2π) the closed interval from $-\Phi(a)$ to $\Phi(a)$. Depending on whether b has a positive or negative imaginary part, we can then obtain $Z-Z_{12}$ negative at the first zero of $Z+Z_{12}$ by either setting $\eta_2=0$ and increasing η_1, or by setting $\eta_1=0$ and increasing η_2, that is, with either $g_2=0$ or $g_1=0$.

B. The case $g=1$

While some of the results below have extensions to the case of general $g>\geqslant 1$, they are mostly of interest for $g=1$, and hence the statements and proofs are restricted to this case.

Lemma 5.6: With f of the form (4.1) satisfying the Lee–Yang condition, the first zero of Z_A with $|A|=2$ always occurs for $\zeta<\pi/4$ when $g=1$.

Proof: Suppose that $A=\{1,2\}$. By Theorem 3.7, the first zero can only increase if we set all $g_j=0$ except for $j=1,2$. In this case we have, in the notation of (5.2),

$$Z_{12}=(\cos\eta_1\cos\eta_2)Z^0(\langle\sigma_1\sigma_2\rangle-t_1t_2), \tag{5.7}$$

where $\langle\sigma_1\sigma_2\rangle$—see (5.4) and Lemma 4.4—is positive. On the other hand, as the average of a quantity taking the values ± 1, $\langle\sigma_1\sigma_2\rangle$ is strictly less than 1 when the J_A in (4.1) are noninfinite. Thus $\eta_1=\eta_2=\zeta$ must be less than $\pi/4$ at the first zero of Z_{12}.

An immediate consequence of this lemma and Theorem 4.11 is:

Theorem 5.7: With $g=1$ and the Lee–Yang condition satisfied, the first zero of $Z(\zeta)$, *if it lies in the interval*

$$\pi/4\leqslant\zeta<\pi/2, \tag{5.8}$$

is a strictly decreasing function of each J_A with $|A|=2$.

As noted earlier, as the J_A tend to zero ("high temperature limit"), the zeros of $Z(\zeta)$ in the principal interval move towards $\zeta=\pi/2$, so that Theorem 5.7 may be interpreted as saying that at high enough temperatures the first zero of Z will have the expected dependence on J_A for $|A|=2$. A somewhat analogous "low temperature" (large J_A) result is the following:

Theorem 5.8: With $g=1$ and the Lee–Yang condition satisfied, the first zero of Z is a strictly decreasing function of each J_A with $|A|$ even, *if it lies in the interval*

$$\pi/2n<\zeta<\pi/2(n-2). \tag{5.9}$$

Proof: Note that $\pi/2n$ is the lower limit of the first zero of Z, Lemma 4.5. We shall consider the case $A=\{1,2\}$, as the proof for $|A|\geqslant 4$ is precisely analogous. Note that

$$Z-Z_{12}=\Sigma_\sigma(1-\sigma_1\sigma_2)f(\sigma)\exp(i\zeta\,\Sigma_j\sigma_j), \tag{5.10}$$

and that, just as in the proof of Lemma 4.5, we may write this as a sum of cosines with positive coefficients and arguments which lie between 0 and $(n-2)\zeta$. (The upper limit for the argument differs from that in Lemma 4.5 because the terms with $\sigma=+1,\sigma=-1$ vanish.) Hence $Z-Z_{12}$ is positive and Z_{12} negative at the first zero of Z if it falls in the interval (5.9). The desired result is thus a consequence of Theorem 4.10.

The lower limit in (5.8) and the upper limit in (5.9) coincide for $n=4$, thus providing a result similar to Theorem 5.4 under the weaker condition $g=1$. But for $n\geqslant 5$ there is a gap between the "high" and "low temperature" intervals, and we have not found an argument which will fill it.

C. Dependence on system size

Let us call a set of sites N, the corresponding interactions J, and the set of g_j values g a "system," and define a subsystem of this system to be N', J', and g' where N' is a subset of N, $J'_A=J_A$ for $A\subset N'$, and $g'_j=g_j$ for $j\in N'$. The function Z' for the subsystem is obtained from the obvious counterpart of (2.1), with the sum restricted to σ_j with $j\in N'$. Alternatively, the original system can be considered "larger" than the subsystem. The expectation that in some cases a sequence of larger and larger systems will have zeros of Z approaching $\zeta=0$ (the Yang and Lee[3] model of a phase transition) suggests making a comparison between the location of zeros of a system and a subsystem. The following are some relatively weak results in this direction. Note that the single site condition of Theorem 5.9 amounts, in graphical terms, to saying that the subsystem is connected to the rest of the system at the single site k; were k deleted, one would have two noninteracting subsystems.

Theorem 5.9: Suppose the system N, J, g satisfies the Lee–Yang condition and has $g>\geqslant 0$. Let N', J', g' be a subsystem as defined above. Suppose, in addition, there is a single site $k\in N'$ with the property that for all $J_A\neq 0$, either $A\subset N'$ or $A\cap N'=\varnothing$ or $A\cap N'=\{k\}$. Then for any $B\subset N'$ (including $B=\varnothing$), the zeros of Z'_B are further from the origin than those of Z_B in the sense that for any $\alpha>0$, there are at least as many zeros of Z_B as of Z'_B in the interval $0\leqslant\zeta\leqslant\alpha$.

Proof: We note that if the g_j with $j\in N\setminus N'$ are all set equal to zero, the zeros of Z_B will move away from $\zeta=0$, Theorem 3.7 (iii). When these g_j are zero, one can show that the sum (2.1) over the σ_j with $j\in N\setminus N'$ is the same when $\sigma_k=+1$ as when $\sigma_k=-1$. Consequently, Z_B is now a constant multiple of Z'_B and has the same zeros.

One can, of course, apply Theorem 5.9 in an iterative manner, and obtain results such as the following:

Corollary 5.10: Given two Cayley trees with ferromagnetic pair interactions (see Corollary 5.2), one of which is larger than the other in the sense defined above, then all the zeros of $Z(\zeta)$ for the larger system are closer to $\zeta=0$ than those of the smaller system.

An example discussed in Sec. VD below [see Example 1(c)] shows that one cannot in general expect results of this generality involving *all* the zeros of Z; in other words, the single site condition plays a nontrivial role in Theorem 5.9. On the other hand, since a subsystem is obtained from a system by setting certain interactions equal to zero, Conjecture 1, if correct, would imply that the *first* zero of Z (*not* Z_B for general B) would decrease monotonically with increasing system size in the case of ferromagnetic pair interactions and $g>\geqslant 0$. Theorem 5.7, which shows that Conjecture 1 is correct at high temperatures, can be used to establish the following result:

Theorem 5.11: Consider a system $N, J, g = 1$ and a subsystem (as defined above) $N', J', g' = 1$. Suppose that the subsystem satisfies the Lee–Yang condition and that if A is a subset of N but not of N', $J_A = 0$, unless $|A| = 2$, in which case $J_A \geqslant 0$. (That is, the system is obtained from the subsystem by "turning on" some ferromagnetic pair interactions.) Then, if ζ is the first zero of Z, ζ' is that of Z', and either $\zeta \geqslant \pi/4$ or $\zeta' \geqslant \pi/4$, it is the case that $\zeta \leqslant \zeta'$.

Proof: We may assume without loss of generality that all sites of the system are connected (in the sense of Sec. IVA), directly or indirectly, to sites of the subsystem, since, if this is not so, Z factors into a contribution from sites having this property (including sites of the subsystem) and the remainder. Repeated applications of Lemma 2.6—see remarks following Lemma 4.3—then show that Z satisfies the Lee–Yang condition, permitting the application of Theorem 5.7.

D. Some specific results for small systems

1. The case n = 4

Consider the case $g = 1$, and assume that the only nonzero J_A are J_{12}, J_{23}, J_{34}, and J_{41}. In terms of the variables

$$\lambda = \cos 2\zeta, \tag{5.11}$$

$$x_{ij} = \exp(-2J_{ij}), \tag{5.12}$$

we have

$$\begin{aligned} Z/2 = 2\lambda^2 &+ (x_{12}x_{23} + x_{23}x_{34} \\ &+ x_{34}x_{41} + x_{41}x_{12})\lambda + (x_{41}x_{23} + x_{12}x_{34} \\ &+ x_{12}x_{23}x_{34}x_{41} - 1), \end{aligned} \tag{5.13}$$

and $Z_{12}/2$ can be obtained from this expression by replacing x_{12} by $-x_{12}$. The zeros of Z and Z_{12} as functions of λ can be calculated explicitly; in addition, $Z - Z_{12}$ has no λ^2 terms, and thus its zero is easily located. Straightforward calculations then yield the following results.

(a) In the case $J_{41} = 0$, the other three J_{ij} strictly positive, the zeros of Z_{12} on the principal interval

$$-1 \leqslant \lambda \leqslant 1 \tag{5.14}$$

intertwine those of Z, with the first zero of Z_{12} as λ decreases from 1 preceding the first zero of Z. Thus both zeros of Z move towards $\lambda = 1$ ($\zeta = 0$) as J_{12} increases, Theorem 4.11.

(b) With $J_{34} = 0$, the other three J_{ij} strictly positive, $Z - Z_{12}$ is positive on the principal interval (5.14), so that the first zero of Z_{12} (as λ decreases from 1) precedes that of Z, but the second zero of Z_{12} follows that of Z. Hence as J_{12} increases, the first zero of Z moves towards $\lambda = 1$ ($\zeta = 0$), but the second moves in the opposite direction. The latter confirms the assertion made just before stating the conjectures in Sec. IVC.

(c) In the case just mentioned, one could imagine increasing the size of the system in the sense of Sec. VC above by the device of adding a site σ_5 with $g_5 = 0$ and $J_{15} = J_{25} > 0$. Carrying out the sum over σ_5, one finds that the result is effectively the same as *increasing* J_{12}, and thus an increase of system size in this case leads to one of the zeros of $Z(\zeta)$ moving to larger rather than smaller ζ. The proof of Theorem 4.12 shows how one could construct an example with the same property, but $g = 1$. This shows that the single site condition of Theorem 5.9, obviously not satisfied in this example, plays a crucial role.

(d) Suppose that $J_{12} = J_{34} = \hat{J} > 0$, $J_{23} = J_{41} > 0$, and denote x_{12} and x_{23} by x and y, respectively. One can show that both zeros of $Z(\zeta)$ move towards $\zeta = 0$ as x decreases ($\hat{J}$ increases) provided

$$x < y\sqrt{2/(1+y^2)}, \tag{5.15}$$

in particular if $x = y$, whereas the second zero of $Z(\zeta)$ moves in the opposite sense if the inequality is reversed. This suggests that only with a rather high degree of symmetry can one expect conclusions as strong as those of Conjecture 2.

(e) Since in case (b) the second zero of Z tends to move towards $\zeta = 0$ (the "right" direction) when J_{41} and J_{23} increase—this follows from noting that J_{41} and J_{23} in case (b) play the same role as J_{12} in case (a)—and only away from $\zeta = 0$ (the "wrong" direction) as J_{12} increases, one might be tempted to suppose that the net motion would be in the right direction if one considered a "change in temperature," that is, the nonzero J_{ij} equal to constants times a parameter β (the inverse temperature). A direct calculation with $J_{41} = J_{23} > J_{12}$ shows that this is *not* the case; when β is small, the second zero moves in the right direction as β increases (hardly surprising, in that it starts at $\pi/2$ when $\beta = 0$), but eventually, when β is sufficiently large, it reverses its direction and thereafter moves the wrong way.

2. An example with n = 9: Zeros of the magnetization

The magnetization for $g = 1$ is equal to $-iZ^{-1}\partial Z/\partial\zeta$, and in view of Theorem 3.6, the zeros of $\partial Z/\partial\zeta$ will determine those of the magnetization. We consider a system with nine sites labeled jk, where both j and k take on the values 1, 2, and 3, and the only nonzero interactions are pair interactions between distinct sites given by

$$J(jk;j'k') = J_1\delta_{jj'} + J_2\delta_{kk'}. \tag{5.16}$$

First consider the situation with $J_2 = 0$, $J_1 > 0$, in which case Z is equal to $\tilde{Z}^3$, where $\tilde{Z}$ is the partition function for three sites with interactions J_1 between all three pairs. It is easy to show that $\tilde{Z}$ has a zero at

$$\cos\zeta_0 = \tfrac{1}{2}\sqrt{3}\sqrt{1 - \exp(-4J_1)}, \tag{5.17}$$

with ζ_0 between 0 and $\pi/2$.

Since $\partial\tilde{Z}/\partial\zeta$ does not vanish, $\partial Z/\partial\zeta$ will have a double zero at $\zeta = \zeta_0$. This is possible because with $J_2 = 0$ the Lee–Yang condition will not be valid for Z. However, for any $J_2 > 0$ the Lee–Yang condition will hold (Lemma 4.2), and this double zero will split into two single zeros, one larger and one smaller than ζ_0 by amounts proportional to $\sqrt{J_2}$ in lowest order. It is clear that the larger zero will increase with increasing J_2 when J_2 is small. Further, if J_1 is extremely large (so that ζ_0 is almost independent of J_1), this behavior will persist over some range of strictly positive J_2 values, even if J_1 and J_2 are simultaneously increased by the same factor (corresponding to a decrease in temperature). Such an "anomalous" dependence on J_2 can also be turned into an "anomalous" dependence on system size using the strategy given above in Sec. VD1(c).

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Generalized two-dimensional O(3) sigma model

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We generalize the two-dimensional O(3) nonlinear σ-model while preserving its conformal invariance. The integrability condition of this model encompasses the sine-Gordon equation in addition to some special cases which are found to be of the same form. The time-independent solutions exhibit solitonlike behavior.

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I. INTRODUCTION

Two-dimensional O(n)-invariant Lagrangian field theories whose field functions describe a homogeneous space have received a lot of attention in the literature. The simplest of these models is the O(3)/O(2) model[1] whose field variable is the three-dimensional unit vector **n**. The Lagrangian density of this theory consists of the scalar product of the first derivatives of this vector. The corresponding action is conformally invariant. It turns out that this model has a number of interesting properties, the most important of which is that its integrability condition is the sine-Gordon equation.[2-4]

In this paper we generalize this model while maintaining its conformal invariance. To this end, we insert into the Lagrangian an arbitrary function of the angle between the light-cone derivatives of **n**. Different choices of this function will lead to different conformally invariant O(3) models.

Starting from this generalized Lagrangian we proceed as follows. The Euler–Lagrange equations of motion, together with the constraint that the norm of **n** is equal to unity, gives us the relation between the function f that modifies the Lagrangian and the magnitudes of the first derivatives of **n**. Making use of this relation and employing the geometrical interpretation of the field vector **n** and its first derivatives, we construct the equation for the angle between the light-cone derivatives of **n**. This integrability condition reduces to the sine-Gordon equation when the function f is taken to be unity.

We examine the time-independent, the space-independent and the Euclidean-invariant versions of this integrability condition. The equations corresponding to the first two cases reduce to the harmonic oscillator equation. The Euclidean-invariant one is the Euclidean sinh-Gordon equation. These three cases, together with the sine-Gordon equation smoothly fit together with a variable transformation.

Finally we examine the time-independent version of this integrability condition. After studying one special case, we devise a procedure for a systematic construction of potentials corresponding to different choices of the function f.

II. THE GENERALIZED σ-MODEL AND ITS INTEGRABILITY CONDITION

Our starting point is the O(3)-invariant chiral theory in one time and one space dimension which is described by the Lagrangian density

$$L = \mathbf{n}_u \cdot \mathbf{n}_v + \lambda(\mathbf{n}^2 - 1). \tag{2.1}$$

The interaction arises form the condition that $\mathbf{n}\cdot\mathbf{n}$ is equal to one. u and v are the light-cone coordinates.

$$u = (t + x)/\sqrt{2}, \qquad v = (t - x)/\sqrt{2}. \tag{2.2}$$

Noting that the angle θ between $\mathbf{n}_u$ and $\mathbf{n}_v$ is a conformally invariant quantity, we propose to generalize the O(3)-invariant theory by modifying the Lagrangian in the following way

$$L = \mathbf{n}_u \cdot \mathbf{n}_v f(\theta) + \lambda(\mathbf{n}^2 - 1). \tag{2.3}$$

The corresponding equation of motion is

$$\mathbf{n}_u \cdot \mathbf{n}_v \frac{\partial f}{\partial z}\frac{\partial z}{\partial \mathbf{n}} + 2\lambda \mathbf{n} = \frac{\partial}{\partial u}\left(\mathbf{n}_v f + (\mathbf{n}_u \cdot \mathbf{n}_v)\frac{\partial f}{\partial z}\frac{\partial z}{\partial \mathbf{n}_u}\right) + \frac{\partial}{\partial v}\left(\mathbf{n}_u f + (\mathbf{n}_u \cdot \mathbf{n}_v)\frac{\partial f}{\partial z}\frac{\partial z}{\partial \mathbf{n}_v}\right), \tag{2.4}$$

where z is defined as

$$z \equiv \tan\theta = \mathbf{n}_u \times \mathbf{n}_v \cdot \mathbf{n}/\mathbf{n}_u \cdot \mathbf{n}_v. \tag{2.5}$$

Multiplying (2.4) by $\mathbf{n}_u$ and making use of the fact that $\mathbf{n}_u$ is orthogonal to **n** due to $\mathbf{n}^2 = 1$, we get an equation of the form

$$\left[\frac{\partial \mathbf{F}}{\partial v} + \frac{\partial \mathbf{G}}{\partial u}\right]\cdot\mathbf{n}_u = 0. \tag{2.6}$$

This can be written as

$$\frac{\partial}{\partial v}(\mathbf{F}\cdot\mathbf{n}_u) + \frac{\partial}{\partial u}(\mathbf{G}\cdot\mathbf{n}_u) - \mathbf{F}\cdot\frac{\partial \mathbf{n}_u}{\partial v} - \mathbf{G}\cdot\frac{\partial \mathbf{n}_u}{\partial u} = 0. \tag{2.7}$$

By elementary manipulations we derive an equation for the norm of $\mathbf{n}_u$:

$$\frac{\partial}{\partial v}\left[|\mathbf{n}_u|^2\left(f - \frac{df}{dz}z\right)\right] = 0, \qquad |\mathbf{n}_u|^2\left(f - \frac{df}{dz}z\right) = G^2(u). \tag{2.8}$$

Similarly, multiplying (2.4) by $\mathbf{n}_v$ leads to

$$\frac{\partial}{\partial u}\left[|\mathbf{n}_v|^2\left(f - \frac{df}{dz}z\right)\right] = 0, \qquad |\mathbf{n}_v|^2\left(f - \frac{df}{dz}z\right) = H^2(v). \tag{2.9}$$

Since our original Lagrangian is form invariant under a local transformation of the form

$$(u,v)\to(u',v'),\qquad du' = |G(u)|\,du,\quad dv' = |H(v)|dv, \tag{2.10}$$

we have

$$|\mathbf{n}_u|^2 = G^2(u)|\mathbf{n}_{u'}|^2,\qquad |\mathbf{n}_v|^2 = H^2(v)|\mathbf{n}_{v'}|^2. \tag{2.11}$$

Making use of the above transformations we may write (2.8) and (2.9) as

$$\left(f-\frac{df}{dz}z\right)|\mathbf{n}_{u'}|^2 = 1,\qquad \left(f-\frac{df}{dz}z\right)|\mathbf{n}_{v'}|^2 = 1, \tag{2.12}$$

or using (2.5)

$$|\mathbf{n}_{u'}|^2 = |\mathbf{n}_{v'}|^2 = \left(f-\frac{df}{d\theta}\sin\theta\cos\theta\right)^{-1} \equiv \gamma(\theta). \tag{2.13}$$

Hereafter we take the transformed coordinates as the basic variables and omit the primes. This transformation yields a Hamiltonian density which vanishes when the constant part is subtracted. This difficulty of correctly defining the energy[5] also arises in the conventional σ-model and can be dealt with using standard methods.

It has been shown by Pohlmeyer that the integrability condition of the dynamical system described by (2.1) leads to the sine-Gordon equation. Here we proceed along similar lines for the Lagrangian (2.3) to find a generalization of the sine-Gordon equation. First we compute the mixed derivative $\mathbf{n}_{uv}$ and the second derivatives $\mathbf{n}_{uu}$ and $\mathbf{n}_{vv}$ in terms of the three basic vectors $\mathbf{n}_u$, $\mathbf{n}_v$, and $\mathbf{n}$ which span R^3. Because of the constraint $\mathbf{n}\cdot\mathbf{n} = 1$, these vectors are linearly independent provided $\mathbf{n}_u\cdot\mathbf{n}_v$ does not vanish.

Then, we note the following equalities:

$$\begin{aligned}
\mathbf{n}_{uv}\cdot\mathbf{n} &= (\mathbf{n}_u\cdot\mathbf{n})_v - \mathbf{n}_u\cdot\mathbf{n}_v = -\gamma\cos\theta,\\
\mathbf{n}_{uv}\cdot\mathbf{n}_u &= \tfrac{1}{2}(\mathbf{n}_u\cdot\mathbf{n}_u)_v = \tfrac{1}{2}\gamma_v,\\
\mathbf{n}_{uv}\cdot\mathbf{n}_v &= \tfrac{1}{2}(\mathbf{n}_v\cdot\mathbf{n}_v)_u = \tfrac{1}{2}\gamma_u,\\
\mathbf{n}_{uu}\cdot\mathbf{n} &= (\mathbf{n}_u\cdot\mathbf{n})_u - \mathbf{n}_u\cdot\mathbf{n}_u = -\gamma,\\
\mathbf{n}_{uu}\cdot\mathbf{n}_u &= \tfrac{1}{2}(\mathbf{n}_u\cdot\mathbf{n}_u)_u = \tfrac{1}{2}\gamma_u,\\
\mathbf{n}_{uu}\cdot\mathbf{n}_v &= (\mathbf{n}_u\cdot\mathbf{n}_v)_u - \mathbf{n}_u\cdot\mathbf{n}_{uv}\\
&= \gamma_u\cos\theta - \gamma\sin\theta\,\theta_u - \tfrac{1}{2}\gamma_v,\\
\mathbf{n}_{vv}\cdot\mathbf{n} &= (\mathbf{n}_v\cdot\mathbf{n})_v - \mathbf{n}_v\cdot\mathbf{n}_v = -\gamma,\\
\mathbf{n}_{vv}\cdot\mathbf{n}_v &= \tfrac{1}{2}(\mathbf{n}_v\cdot\mathbf{n}_v)_v = \tfrac{1}{2}\gamma_v,\\
\mathbf{n}_{vv}\cdot\mathbf{n}_u &= (\mathbf{n}_u\cdot\mathbf{n}_v)_v - \mathbf{n}_{uv}\cdot\mathbf{n}_v\\
&= \gamma_v\cos\theta - \gamma\sin\theta\,\theta_v - \tfrac{1}{2}\gamma_u.
\end{aligned} \tag{2.14}$$

Making use of the above expressions we obtain

$$\begin{aligned}
\mathbf{n}_{uv} &= -\gamma\cos\theta\,\mathbf{n}\\
&\quad + \frac{1}{2\gamma}\left[\gamma_v - \left(\frac{\gamma_u - \gamma_v\cos\theta}{\sin^2\theta}\right)\cos\theta\right]\mathbf{n}_u\\
&\quad + \frac{1}{2\gamma}\left(\frac{\gamma_u - \gamma_v\cos\theta}{\sin^2\theta}\right)\mathbf{n}_v,\\
\mathbf{n}_{uu} &= -\gamma\mathbf{n}\\
&\quad + \frac{1}{2\gamma}\left[\gamma_u - \left(\frac{\gamma_u\cos\theta - 2\gamma\sin\theta\,\theta_u - \gamma_v}{\sin^2\theta}\right)\cos\theta\right]\mathbf{n}_u\\
&\quad + \frac{1}{2\gamma}\left(\frac{\gamma_u\cos\theta - 2\gamma\sin\theta\,\theta_u - \gamma_v}{\sin^2\theta}\right)\mathbf{n}_v,\\
\mathbf{n}_{vv} &= -\gamma\mathbf{n}\\
&\quad + \frac{1}{2\gamma}\left(\frac{\gamma_v\cos\theta - 2\gamma\sin\theta\,\theta_v - \gamma_u}{\sin^2\theta}\right)\mathbf{n}_u\\
&\quad + \frac{1}{2\gamma}\left[\gamma_v - \left(\frac{\gamma_v\cos\theta - 2\gamma\sin\theta\,\theta_v - \gamma_u}{\sin^2\theta}\right)\cos\theta\right]\mathbf{n}_v.
\end{aligned} \tag{2.15}$$

Next we substitute these vectors into the identity

$$\mathbf{n}_{uv}\cdot\mathbf{n}_{uv} = \tfrac{1}{2}(\mathbf{n}_u^2)_{vv} + \tfrac{1}{2}(\mathbf{n}_v^2)_{uu} - (\mathbf{n}_u\cdot\mathbf{n}_v)_{uv} + \mathbf{n}_{uu}\cdot\mathbf{n}_{vv}. \tag{2.16}$$

The resulting expression yields a generalized version of the sine-Gordon equation in light-cone coordinates.

$$\begin{aligned}
&2\gamma\sin\theta(\gamma\sin\theta + \theta_{uv})\\
&\quad + (\theta_u^2 + \theta_v^2 - 2\theta_u\theta_v\cos\theta)(\gamma'' - \gamma'^2/\gamma)\\
&\quad - (\theta_u^2\cos\theta + \theta_v^2\cos\theta - 2\theta_u\theta_v)(\gamma'/\sin\theta)\\
&\quad + (\theta_{uu} + \theta_{vv} - 2\theta_{uv}\cos\theta)\gamma' = 0.
\end{aligned} \tag{2.17}$$

This equation is the integrability condition of the equations of motion of the Lagrangian (2.3). A choice of the function $\gamma = \gamma(\theta)$, through Eq. (2.13) determines the specific form of the Lagrangian. In contrast to the sine-Gordon case which is given by $\gamma =$ const this equation is not Lorentz invariant in the general case. This is expected since a conformal transformation has already been performed in (2.10). It follows that the Lorentz invariance of the integrability condition for the standard σ-model is the result of the specific choice $\gamma =$ const. In the next section we will show that there is a one-parameter family of generalized σ-model Lagrangians for which Eq. (2.17) after a transformation of variables again leads to the sine-Gordon equation.

III. SPECIAL CASES EXHIBITING SYMMETRIES

In this section, we search for certain choices of γ which will reduce (2.17) to a system with some kind of additional symmetry. Therefore, we first look for an expression for γ which will render (2.17) Lorentz invariant. The only choice is readily seen to be $\gamma =$ const, which gives the sine-Gordon equation.

Next we try to make (2.17) Euclidean invariant. To this end, we separate the terms that multiply the mixed derivatives $\theta_u\theta_v$ and θ_{uv}. They are

$$\cos\theta(\gamma'' - \gamma'/\sin\theta\cos\theta - \gamma'^2/\gamma), \tag{3.1}$$

$$\gamma'\cos\theta - \gamma\sin\theta, \tag{3.2}$$

respectively.

We note that when γ equals $c^2/|\cos\theta|$ both (3.1) and (3.2) are zero. Substituting this value for γ in (2.17) we get an Euclidean-invariant equation

$$2c^2\sin\theta + (\theta_u^2 + \theta_v^2)\tan\theta + (\theta_{uu} + \theta_{vv}) = 0. \tag{3.3}$$

We multiply this equation by an integrating factor η'. When η' equals $1/\cos\theta$, (3.3) reduces to

$$\eta_{uu} + \eta_{vv} + 2c^2 \sinh \eta = 0\,, \tag{3.4}$$

where the "potential" is

$$V(\eta) = 2c^2 \cosh \eta\,. \tag{3.5}$$

Another simple case reveals itself when we impose $x \to x' = f(x)$ symmetry. In other words, we require that the integrability condition be x-independent. Going back to one-space and one-time coordinates it is seen that (2.17) can be written as

$$2\gamma \sin\theta + [\theta_t((\gamma'/\gamma)\tan(\theta/2) + 1)]_t - [\theta_x(1 - (\gamma'/\gamma)\cot(\theta/2))]_x = 0\,. \tag{3.6}$$

When γ equals $c^2/(1 + \cos\theta)$, (3.6) reduces to

$$c^2(\tan(\theta/2)) + [\theta_t \tfrac{1}{2}(\sec^2(\theta/2))]_t = 0\,. \tag{3.7}$$

Defining $\tan(\theta/2)$ as η, we get the harmonic oscillator equation

$$c^2\eta + \eta_{tt} = 0\,. \tag{3.8}$$

For this case we note that the tangent of the angle between the vectors $\mathbf{n}_u$ and $\mathbf{n}_v$ oscillate in time with a period proportional to the norm of these vectors.

We proceed along similar lines to get the time-independent version of (3.6). When γ is $c^2/(1\text{-}\cos\theta)$, (3.6) becomes

$$c^2(\cot(\theta/2)) + [\theta_x(-\tfrac{1}{2}\csc^2(\theta/2))]_x = 0\,. \tag{3.9}$$

Letting $\cot(\theta/2)$ be defined as η yields the harmonic oscillator equation for η,

$$c^2\eta + \eta_{xx} = 0\,. \tag{3.10}$$

This time the oscillation is in space.

Using Eq. (2.13) which shows the relation between γ and f, we can summarize our results as follows. When the Lagrangian density is given by (2.1), the integrability condition is Lorentz invariant; it yields the sine-Gordon equation, a well-known result. However, when $+(-)\,|\mathbf{n}_u|\,|\mathbf{n}_v|$ is added to the Lagrangian density, the corresponding integrability condition becomes time (space) independent and reduces to the harmonic oscillator equation. Finally $\mathbf{n}_u \cdot \mathbf{n}_v$ replaced by $|\mathbf{n}_u|\,|\mathbf{n}_v|$ gives the Euclidean-invariant integrability condition, or the Euclidean sinh-Gordon equation.

All these four cases can be unified with a variable transformation as follows. Looking back at Eq. (3.6) we define

$$\eta' = (\gamma'/\gamma)\tan(\theta/2) + 1\,. \tag{3.11a}$$

$$\xi' = 1 - (\gamma'/\gamma)\cot(\theta/2)\,. \tag{3.11b}$$

Hence (3.6) can be written as

$$2\gamma \sin\theta + \eta_{tt} - \xi_{xx} = 0\,. \tag{3.12}$$

The simplest relation between η and ξ would be

$$\eta = a^2\xi\,, \tag{3.13}$$

where a^2 is a constant. In order to satisfy (3.13) γ and f have to take the special values

$$\gamma = c^2|(a^2 + 1) + (a^2 - 1)\cos\theta|^{-1}\,, \tag{3.14}$$

$$f = c^{-2}|a^2 + 1 + (a^2 - 1)/\cos\theta|\,. \tag{3.14}$$

Disregarding an overall constant, these determine a family of Lagrangians depending on the parameter a. Substituting this in (3.11a) we get

$$a\tan(\eta/2a) = \tan(\theta/2)\,. \tag{3.15}$$

Using this as the definition of η, (3.12) reduces to

$$c^2 \sin(\eta/a) + a\eta_{tt} - (1/a)\eta_{xx} = 0\,. \tag{3.16}$$

Rescaling η and our time (or x) coordinates we get the sine-Gordon equation for η. Furthermore from (3.14) we can see that when a^2 is positive, negative, zero, or infinity we get the sine-Gordon, the Euclidean sinh-Gordon, the time-independent or the x-independent equations, respectively. So all four cases are unified when we impose (3.13) upon our integrability condition.

IV. BEHAVIOR OF TIME-INDEPENDENT SOLUTIONS

In this section we consider only the time-independent solutions of (3.6) which are given by

$$2\gamma \sin\theta - [\theta_x(1 - (\gamma'/\gamma)\cot(\theta/2))]_x = 0\,. \tag{4.1}$$

Before we set up a procedure for finding solutions systematically, we consider one special case. We try γ of the form

$$\gamma = a^2(1 + \cos\theta)^b\,. \tag{4.2}$$

Substituting this in (4.1) we get the potential

$$\tfrac{1}{2}\theta_x^2 = (2/(1+b)^2)(c^2 - a^2(1 + \cos\theta)^{1+b})\,, \tag{4.3}$$

where c^2 is a constant of integration. We can put (3.3) in a closed form for x by letting u equal $\tan(\theta/2)$,

$$x = (1+b)\int^{\tan\theta/2} du(c^2(1+u^2)^2 - a^2 2^{b+1}(1+u^2)^{1-b})^{-1/2}\,. \tag{4.4}$$

We first note that $b = -1$ will make x equal 0. This case corresponds to the x-independent case of Sec. III. We recover the sine-Gordon limit when b equals 0. So the next simple case is given by b equals 1. We get

$$x = (2/c)\{(1/g)F(\alpha,q)\}\,, \tag{4.5}$$

where

$$q = 2\sqrt{a(2a+c)^{-1}}\,,\quad g = \sqrt{(2a+c)/c}\,,$$

$$\tan\alpha = \tan(\theta/2)\sqrt{(c-2a)^{-1}c}\,,$$

and F is an elliptic integral of the first kind. Still another manifestly integrable case is $b = -2$. This yields x as a linear combination of elliptic integrals of the first and third kinds. These solutions can be compared to the time-independent solution of the sine-Gordon equation which is an elliptic integral of the first kind.

In order to find out which function f in the Lagrangian would give these solutions, we go back and solve (2.13) and get

$$f(\theta) = 3/4a^2 - 1/(4a^2\cos\theta) - (1-\cos\theta)^2/[12a^2\cos\theta(1+\cos\theta)] \tag{4.6}$$

when $b = 1$.

Going on to the general case, we note that when we let

$$\eta' = (1 - (\gamma'/\gamma)\cot(\theta/2))\,, \tag{4.7}$$

$2\gamma\sin\theta$ term in (4.1) can be written as

$$- 2c\frac{d}{d\eta}(\gamma(1 + \cos\theta)) . \tag{4.8}$$

Identifying $2c\gamma(1 + \cos\theta)$ with the potential we write (4.1) as

$$\tfrac{1}{2}\eta_x^2 + V(\eta) = c . \tag{4.9}$$

Going back to the Eq. (4.7) we note, after integration,

$$\eta = \theta - \int^{\theta} \frac{\gamma'}{\gamma} \cot\Big(\frac{\phi}{2}\Big) d\phi . \tag{4.10}$$

We can extract some information from this equation. We immediately notice that the sine-Gordon limit, where γ is a constant gives $\eta = \theta$. Furthermore, when γ equals $c/(1 + \cos\theta)$, (4.1) becomes x independent, as we realized before. This gives $\eta = 0$ as expected.

$\gamma(\theta)$ must be an even, periodic function of θ if the Lagrangian is to be parity invariant. Hence, the integrand in (4.10) must be even. When integrated it will, in general, give another term proportional to θ plus an odd, periodic function of θ. Therefore, in general, by rescaling η if necessary, η and θ differ by an odd, periodic function. In this case any periodic function of θ, when expressed as a function of η is again periodic. Hence the potential $V(\eta)$ in (4.9) is periodic and the time-independent solutions will exhibit solition behavior. In cases where γ is chosen such that the term proportional to θ in Eq. (4.10) cancels, η will be a periodic function of θ, and $V(\eta)$ is not necessarily periodic in η. Then the time-independent solutions need not exhibit soliton behavior. The Euclidean sinh-Gordon equation provides an example for this case.

V. CONCLUSION

We have constructed a family of classical two-dimensional O(3) σ-models whose integrability condition is a generalization of the sine-Gordon equation. Searching for special cases of this equation which exhibit symmetries we have found a one-parameter family of Lagrangians whose integrability condition is again given by the sine-Gordon equation. At special values of this parameter the integrability condition abruptly changes from the sine-Gordon equation to the Euclidean sinh-Gordon equation, whereas at precisely these special values the equation becomes either the time-independent or the x-independent one-dimensional harmonic oscillator equation. Thus the physical behavior of the system undergoes a change at these special values of the parameter. This suggests that if the system is quantized with this parameter as a coupling constant there is a phase transition at these special values.

Going back to the general case, we have shown that the time-independent solutions in general, but not always, exhibit solitary waves. In some special cases these solutions, just like the solitons of the sine-Gordon equation, are described by elliptic functions.

It has been shown that the sine-Gordon equation also arises in the embedding problem of a two-dimensional surface of constant Riemannian curvature in a three-dimensional Euclidean space.[6] Our preliminary investigations show that the integrability condition (2.17) can be analyzed in the same framework and this equation can be obtained as one of the Gauss–Codazzi equations of a similar embedding problem. Detailed investigations in this direction and attempts to quantize the Lagrangian (2.3) for the specific choice (3.14) seem to be fruitful directions for further research.

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Inverse scattering variables of the KdV equation from the point of view of Galilean mechanics

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The Galilean invariance of the Korteweg–de Vries equation is applied in order to characterize the structure of degrees of freedom displayed by the inverse scattering transform method. It is found that the dynamical systems associated with the discrete scattering data variables admit a description in terms of mass, position, and momentum variables similar to the systems of free Galilean particles. On the other hand, the radiation component of the KdV field associated with the continuous part of the set of scattering data turns out to be described by a new field evolving according to a linear partial differential equation.

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I. INTRODUCTION

In two previous papers,[1,2] we have analyzed the nonlinear Schrödinger equation and the sine-Gordon equation by combining techniques of inverse scattering transform (IST) and Lie group theory. The application of the IST method to these equations reveals a simple structure for their sets of degrees of freedom which separate into a discrete and a continuous part. Our aim was to investigate how the corresponding dynamical systems can be characterized by means of invariance Lie groups. In both cases, the following interpretation was obtained.

(i) Discrete degrees of freedom associated with solitons and breathers describe free particles.

(ii) The radiation component of the nonlinear field determines a new field which transforms under the invariance group according to a linear realization.

The object of the present paper is the analysis of the Korteweg–de Vries (KdV) equation

$$v_t = -v_{xxx} + 6vv_x, \tag{1.1}$$

considered as a Galilean-invariant dynamical system. Indeed, the KdV equation is invariant under the transformations[3]

$$v'(t',x') = v(t,x) - \tfrac{1}{6}c, \tag{1.2}$$

where $x' = x + ct + a$ and $t' = t + b$. Since the work of Gardner, Green, Kruskal, and Miura,[4] it is known that the KdV flow acquires a simple form when expressed in terms of scattering data of the Schrödinger spectral problem. An interpretation of this fact was provided by Faddeev and Zakharov[5] who realized that, from the point of view of Hamiltonian mechanics,[6] the scattering data are essentially a set of action-angle variables. These properties of the KdV equation apply for space V of initial data $v(x)$ verifying $v(x) \to 0$ as $x \to \pm\infty$. The Galilean transformations (1.2) with $c \neq 0$ do not preserve this boundary condition and therefore they are not defined on V. Nevertheless, (1.2) determines a representation of the generators of the extended Galilei group by means of functionals $\{M,H,P,K\}$ which are well defined on V. The Poisson bracket relations satisfied by these functionals reproduce the structure of the extended Galilei Lie algebra with the exception of the Poisson bracket between M and K which is not defined. In spite of this drawback, we adopt this singular representation of the extended Galilei Lie algebra as the basis of our discussion.

The scattering data variables provided by the IST method allow us to analyze the structure of the Galilean generators for the KdV equation by means of concepts of classical Galilean mechanics. The expressions for the functionals M, H, and P in terms of these variables were already calculated by Faddeev and Zakharov.[5] We find here the corresponding expression for the generator K of pure Galilean transformations.

$$K = -\frac{1}{6}\int_{-\infty}^{\infty} xv(x)dx. \tag{1.3}$$

It is worth mentioning that in the derivation of this result, the second symplectic structure of the KdV equation plays a key role. The characterization of the Galilean generators in terms of scattering data variables leads to the following properties.

(i) Discrete scattering data variables support dynamical systems which admit Galilean position and momentum variables and which evolve in time according to the free-particle motion. However, a complete identification of these systems with free classical Galilean particles is not possible due to the different role played by the mass variables.

(ii) Degrees of freedom associated with the continuous scattering data variables determine a new field $u = u(x)$ which under the KdV flow evolves according to the linear evolution equation.

$$u_t = -u_{xxx}. \tag{1.4}$$

These results, together with their analogs for the nonlinear Schrödinger equation and the sine-Gordon equation, provide a group-theoretic interpretation of the dynamical structures exhibited by the IST method. This interpretation, based on the theory of canonical realizations of Lie groups, presents the above-mentioned nonlinear fields as a composition of free particles and linear radiation fields. In this sense, it would be interesting to investigate whether a similar characterization may be formulated in the context of

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the quantum IST through the theory of unitary representations of Lie groups.

II. THE GENERATOR OF GALILEAN TRANSFORMATIONS

A. Scattering data and symplectic forms

We begin by introducing some notation and some basic results about the Schrödinger spectral problem

$$(-\partial_{xx}+v(x))f(k,x)=k^2 f(k,x), \quad -\infty<x<\infty, \tag{2.1}$$

with a potential $v(x)$ satisfying the appropriate decaying conditions so as to assure the existence of the IST.[7,8] Let $f_\pm$ denote the Jost solutions of (2.1) determined by the asymptotic conditions

$$e^{\mp ikx}f_\pm(k,x)=1+o(1), \quad \text{as } x\to\pm\infty. \tag{2.2}$$

These solutions exist for Im $k\geqslant 0$, and for each x, they are analytic in Im $k>0$ and continuous in Im $k\geqslant 0$. For real $k\neq 0$, there exists two functions $a(k)$ and $b(k)$ such that they verify

$$f_+(k,x)=a(k)f_-(-k,x)+b(k)f_-(k,x), \tag{2.3}$$

and

$$a^*(k)=a(-k), \quad b^*(k)=b(-k),$$
$$|a(k)|^2-|b(k)|^2=1. \tag{2.4}$$

The function $a(k)$ may be continued analytically into Im $k>0$ and it has the following asymptotic forms[7,8]:

$$a(k)=-\alpha/k+\beta+o(1), \quad \text{as} \quad k\to 0, \tag{2.5a}$$
$$a(k)=1+\gamma/k+o(1/k), \quad \text{as} \quad k\to\infty, \tag{2.5b}$$

where the coefficients α, β, and γ are

$$\alpha=\frac{1}{2i}\int_{-\infty}^{\infty}v(x)f_+(0,x)dx,$$
$$\beta=1-\frac{1}{2i}\int_{-\infty}^{\infty}v(x)(\dot f_+(0,x)-ixf_+(0,x))dx, \tag{2.6}$$
$$\gamma=\frac{i}{2}\int_{-\infty}^{\infty}v(x)dx.$$

Here, and henceforth, the dot means differentiation with respect to the k variable. The function $a(k)$ possesses a finite number of simple zeros k_l $(l=1,\dots,N)$ which are located on the imaginary axis. It will be assumed that $|k_1|>|k_2|>\cdots>|k_N|$. At each zero k_l, the Jost functions f_+ and f_- are proportional, and we will denote by b_l $(l=1,\dots,N)$ the corresponding real coefficients satisfying

$$f_+(k_l,x)=b_l f_-(k_l,x). \tag{2.7}$$

It is also proved easily that the eigenvalues of the Schrödinger operator coincide with the squared zeros k_l^2 of $a(k)$.

The function $b(k)$ has the asymptotic forms[7,8]

$$b(k)=\alpha/k+\theta+o(1), \quad \text{as} \quad k\to 0, \tag{2.8a}$$
$$b(k)=o(1/k), \quad \text{as} \quad k\to\pm\infty, \tag{2.8b}$$

where α is the same as in (2.5a), and θ is given by

$$\theta=\frac{1}{2i}\int_{-\infty}^{\infty}v(x)(\dot f_+(0,x)+ixf_+(0,x))dx. \tag{2.9}$$

Additional regularity and decaying properties of $a(k)$ and $b(k)$ may be stated for sufficiently differentiable and rapidly decreasing potentials.[9]

One of the most remarkable properties of the IST associated with the Schrödinger spectral problem was discovered by Faddeev and Zakharov,[5] who realized that the Poisson bracket operation

$$\{F,G\}=\int_{-\infty}^{\infty}\frac{\delta F}{\delta v(x)}\partial_x\frac{\delta G}{\partial v(x)}dx, \tag{2.10}$$

introduced by Gardner[6] in connection with the KdV equation, derives from a symplectic form in which the spectral data are essentially a set of action-angle variables. Indeed, as Faddeev and Zakharov proved, this symplectic form is given by

$$\Omega=\sum_l d\eta_l\wedge d\xi_l+\int_0^{\infty}dp(k)\wedge dq(k)dk, \tag{2.11}$$

where

$$\xi_l=2\ln|b_l|, \quad \eta_l=-k_l^2, \quad (l=1,\dots,N), \tag{2.12a}$$
$$q(k)=-\arg b(k), \quad p(k)=(2k/\pi)\ln|a(k)|^2 \quad (k>0). \tag{2.12b}$$

The origin of this simple structure is related to two facts. The first one is the form of the variational derivatives of the scattering data with respect to the potential function[10]

$$\frac{\delta k_l^2}{\delta v(x)}=\psi_l(x)^2, \quad \frac{\delta\ln b_l}{\delta v(x)}=\frac{-i}{2k_l\dot a(k_l)}$$
$$\times[f_-(k_l,x)\dot f_+(k_l,x)-\dot f_-(k_l,x)f_+(k_l,x)], \tag{2.13a}$$

$$\frac{\delta a(k)}{\delta v(x)}=\frac{i}{2k}f_+(k,x)f_-(k,x),$$
$$\frac{\delta b(k)}{\delta v(x)}=-\frac{i}{2k}f_+(k,x)f_-(k,x), \tag{2.13b}$$

where $\psi_l(x)$ in the first equation of (2.13a) denotes the normalized real eigenfunction corresponding to the eigenvalue k_l^2. The second one is that the equations

$$(J_v-k^2\partial_x)fg=0, \tag{2.14a}$$
$$(J_v-k^2\partial_x)(\dot fg-\dot gf)+k(f\partial_x g-g\partial_x f)=0, \tag{2.14b}$$

where

$$J_v=-\tfrac14\partial_{xxx}+v(x)\partial_x+\tfrac12 v_x(x), \tag{2.15}$$

are satisfied for every pair f, g of solutions of (2.1). These equations lead to simple expressions for the Poisson bracket relations among scattering data.

The operator J_v defined in (2.15) is an important object in the analysis of the symplectic properties of the IST. In fact, it defines another Poisson bracket operation according to[11]

$$\{F,G\}'=\int_{-\infty}^{\infty}\frac{\delta F}{\delta v(x)}J_v\frac{\delta G}{\delta v(x)}dx. \tag{2.16}$$

As a consequence of (2.12) and (2.14) we have that

$$(J_v+\eta_l\partial_x)\left(\frac{\delta\xi_l}{\delta v(x)},\frac{\delta\eta_l}{\delta v(x)}\right)=(0,0), \tag{2.17a}$$

$$(J_v - k^2\partial_x)\left(\frac{\delta q(k)}{\delta v(x)},\frac{\delta p(k)}{\delta v(x)}\right) = (0,0). \tag{2.17b}$$

From (2.16), (2.17), and the expression of the symplectic form Ω, one deduces at once that the Poisson bracket $\{\ ,\ \}'$ derives from the symplectic form

$$\Omega' = \sum_l -\frac{1}{\eta_l} d\eta_l \wedge d\xi_l + \int_0^\infty \frac{1}{k^2} dp(k)\wedge dq(k)dk. \tag{2.18}$$

In the subsequent discussion, both symplectic structures Ω and Ω' will be required.

B. The Galilean generator in terms of scattering data

Let us consider the Hamiltonian vector field corresponding to the functional

$$K_0 = \int_{-\infty}^{\infty} xv(x)dx \tag{2.19}$$

under the symplectic structure Ω'. It is defined by[12]

$$\delta v(x) = J_v \frac{\delta K_0}{\delta v(x)} = v + \frac{1}{2}xv_x. \tag{2.20}$$

The derivative of a functional F in the direction of the vector field δv adopts the form

$$\delta F = \int_{-\infty}^{\infty} \frac{\delta F}{\delta v(x)}\delta v(x)dx = \{F,K_0\}'. \tag{2.21}$$

Now we are going to show how a Lax's pair trick enables us to find the derivatives of the scattering data in the direction of δv and, consequently, the Poisson bracket relations between K_0 and the scattering data.

Let $L_v = -\partial_{xx} + v(x)$ denote the Schrödinger operator. A simple calculation shows that

$$\delta v = [\tfrac{1}{2}x\partial_x, L_v] + L_v. \tag{2.22}$$

Hence if we consider the derivative of (2.1) in the direction of δv, and taking into account that

$$k^2 \dot f = (L_v - k^2)\tfrac{1}{2}k\dot f, \tag{2.23}$$

we find

$$(L_v - k^2)(\delta f + \tfrac{1}{2}(k\partial_k - x\partial_x)f) = 0. \tag{2.24}$$

In particular, the asymptotic properties of the Jost solution $f_+(k,x)$ and (2.24) imply that

$$\delta f_+ = \tfrac{1}{2}(x\partial_x - k\partial_k)f_+, \tag{2.25}$$

and, as a consequence, one obtains

$$(\delta k_l,\delta b_l,\delta a(k),\delta b(k)) = (\tfrac{1}{2}k_l, 0, -\tfrac{1}{2}k\dot a(k), -\tfrac{1}{2}k\dot b(k)), \tag{2.26}$$

or, equivalently,

$$(\delta\xi_l,\delta\eta_l,\delta q(k),\delta p(k)) = \left(0,\eta_l, -\frac{1}{2}k\dot q(k), -\frac{1}{2}k^2\frac{d}{dk}(k^{-1}p(k))\right). \tag{2.27}$$

Therefore from (2.21) and the expression of the symplectic form Ω' we deduce that K_0 must satisfy the following equations:

$$\frac{\partial K_0}{\partial \xi_l} = 1, \quad \frac{\partial K_0}{\partial \eta_l} = 0, \tag{2.28a}$$

$$\frac{\delta K_0}{\delta q(k)} = \frac{1}{2}\frac{d}{dk}\left(\frac{p(k)}{k}\right), \quad \frac{\delta K_0}{\delta p(k)} = -\frac{1}{2}\frac{\dot q(k)}{k}. \tag{2.28b}$$

The solution of this system is

$$K_0 = \sum_l \xi_l - \int_0^\infty \frac{1}{2k}\dot q(k)p(k)dk \tag{2.29a}$$

or, equivalently,

$$K_0 = 2\sum_l \ln|b_l| + \frac{1}{\pi}\int_0^\infty \ln|a(k)|^2 \frac{d}{dk}\arg b(k)dk. \tag{2.29b}$$

We make several remarks about Eqs. (2.29): (i) Let us examine the integral terms in Eqs. (2.29). Due to (2.5a) and (2.8a), we have that

$$|a(k)|^2 = -\frac{\alpha^2}{k^2} + o\left(\frac{1}{k^2}\right),$$
$$\arg b(k) = \arg\alpha - i\frac{\theta}{\alpha}k + o(k),$$
$$\text{as } k \to 0+. \tag{2.30}$$

Hence the integrand has a singularity[13] at $k = 0$ and the integral must be considered as the limit of the integral over $k \geqslant \epsilon$ as $\epsilon \to 0+$. According to (2.30), we deduce

$$\ln|a(k)|^2(\arg b(k) - \arg\alpha) = o(1), \quad \text{as} \quad k \to 0+. \tag{2.31}$$

Therefore by integrating by parts

$$\int_0^\infty \ln|a(k)|^2\frac{d}{dk}\arg b(k)dk = -\int_0^\infty \frac{d}{dk}\ln|a(k)|^2\cdot(\arg b(k) - \arg\alpha)dk. \tag{2.32}$$

The last integral in (2.32) is convergent since

$$\frac{d}{dk}\ln|a(k)|^2\cdot(\arg b(k) - \arg\alpha) = 2i\frac{\theta}{\alpha} + o(1), \quad \text{as} \quad k \to 0+. \tag{2.33}$$

This proves that the integral term in Eqs. (2.29) is well defined.

(ii) From (2.4) and (2.5a), it follows that the coefficient α is purely imaginary and then $q(k) = -\arg b(k)$ tends to $\pm\pi/2$ as $k \to 0+$. Consequently, and taking (2.32) into account, it is clear that the expression (2.29a) for K_0 satisfies the two equations of (2.28b).

(iii) Formally, the conditions (2.28) determine K_0 uniquely up to a constant term. Thus the form (2.29a) for K_0 derives from the fact that Eq. (2.29a) holds for $v(x) \equiv 0$. An independent proof of (2.29) for the class of reflectionless potentials is given in the Appendix.

(iv) In the derivation of (2.29) the symplectic form Ω' has been used instead of Ω because this latter leads to a Hamiltonian vector field for $K_0(\delta v(x) = 1)$ whose associated flow does not preserve the asymptotic conditions imposed on the potential functions.

III. GALILEAN OBSERVABLES FOR THE KdV EQUATION

A. The singular realization of the extended Galilei Lie algebra

A Hamiltonian dynamical system, invariant under the Galilei group in two-dimensional space-time, determines a realization of the Lie algebra $\{\hat{M},\hat{H},\hat{P},\hat{K}\}$ of the extended Galilei group by means of four functions $\{M,H,P,K\}$ in the phase space such that

$$\{H,P\}=0,\quad \{H,K\}=P,\quad \{P,K\}=M, \tag{3.1a}$$

$$\{H,M\}=\{P,M\}=\{K,M\}=0. \tag{3.1b}$$

For the KdV equation (1.1) with the Poisson bracket structure $\{\ ,\ \}$, there are four functionals:

$$M=\frac{1}{6}\int_{-\infty}^{\infty} v\,dx,\quad H=\int_{-\infty}^{\infty}\left(\frac{1}{2}v_x^2+v^3\right)dx, \tag{3.2a}$$

$$P=-\frac{1}{2}\int_{-\infty}^{\infty} v^2\,dx,\quad K=-\frac{1}{6}\int_{-\infty}^{\infty} xv\,dx, \tag{3.2b}$$

which satisfy relations (3.1). Nevertheless, according to the definition (2.10) of $\{\ ,\ \}$, the Poisson bracket $\{M,K\}$ is divergent while $\{K,M\}$ vanishes. That is to say, the pair (M,K) does not belong to the domain of pairs of functionals on which $\{\ ,\ \}$ is well defined as a skew-symmetric operation. In spite of this inconvenience we are going to see how the "singular" realization (3.2) of the extended Galilei Lie algebra allows us to define some typical Galilean mechanical variables.

The expressions for M, H, and P in terms of scattering data were already found by Faddeev and Zakharov.[5] With the inclusion of the expression for K that we have deduced in Sec. II, the list of the four functionals is as follows:

$$M=-\frac{2}{3}\sum_l \eta_l^{1/2}+\frac{1}{6}\int_0^{\infty}\frac{1}{k}p(k)dk, \tag{3.3a}$$

$$P=-\frac{8}{3}\sum_l \eta_l^{3/2}-2\int_0^{\infty} kp(k)dk, \tag{3.3b}$$

$$H=-\frac{32}{5}\sum_l \eta_l^{5/2}+8\int_0^{\infty} k^3p(k)dk, \tag{3.3c}$$

$$K=-\frac{1}{6}\sum_l \xi_l+\frac{1}{12}\int_0^{\infty}\dot{q}(k)\,p(k)dk. \tag{3.3d}$$

Each functional is a sum of two different terms depending, respectively, on the discrete and on the continuous parts of the set of scattering data. Observe that the contribution of the continuous part vanishes if and only if $v(x)$ is a reflectionless potential.

B. Discrete degrees of freedom

Let us introduce the canonically conjugate variables

$$q_l=-\tfrac{1}{4}\xi_l\,\eta_l^{-1/2},\quad p_l=-\tfrac{8}{3}\eta_l^{3/2}. \tag{3.4}$$

Then if we denote

$$m_l=-\tfrac{2}{3}\eta_l^{1/2}=(\tfrac{1}{9}p_l)^{1/3}, \tag{3.5}$$

the contributions of the discrete scattering data variables to the Galilean generators take the form

$$M_d=-\frac{2}{3}\sum_l \eta_l^{1/2}=\sum_l m_l, \tag{3.6a}$$

$$P_d=-\frac{8}{3}\sum_l \eta_l^{3/2}=\sum_l p_l, \tag{3.6b}$$

$$H_d=-\frac{32}{5}\sum_l \eta_l^{5/2}=\sum_l\left(\frac{p_l^2}{2m_l}+\frac{81}{10}m_l^5\right), \tag{3.6c}$$

$$K_d=-\frac{1}{6}\sum_l \xi_l=-\sum_l m_l\,q_l. \tag{3.6d}$$

Though these expressions seem to correspond to the Galilean realization of a system of free classical particles, the identification with this system is not complete since the variables m_l, representing the masses of the particles, do not have null Poisson bracket relations with the Galilean generators. In fact, we have that $\{q_l,m_{l'}\}=-2\cdot 3^{-3}\cdot m_l^{-2}\cdot\delta_{ll'}$ and therefore

$$\{m_l,K_d\}=-\tfrac{2}{27}m_l^{-1}. \tag{3.7}$$

However, the dynamical law associated with (3.6) is identical to the one for a system of free particles, i.e.,

$$\frac{dq_l}{dt}=\{q_l,H_d\}=\frac{p_l}{m_l},\quad \frac{dp_l}{dt}=\{p_l,H_d\}=0, \tag{3.8}$$

with the momentum variables p_l having the usual form of mass times velocity. It must be observed that, according to (3.4) and (3.5), the variables p_l and m_l are always negative and consequently the velocities are positive.

For the case of reflectionless potentials, there are closed formulas[14] expressing the potential function $v(x)$ in terms of the discrete scattering data variables. It is easy to find the form that these formulas acquire when the Galilean variables (m_l,q_l,p_l) are used. Thus for a potential with N bound states, it follows that

$$v(x)=-2\partial_{xx}\ln\det(\mathbb{1}+C), \tag{3.9}$$

where C is the $N\times N$ matrix with elements

$$C_{ll'}=-2\frac{\sqrt{m_l m_{l'}}}{m_l+m_{l'}}\times\exp\left[\frac{3}{2}m_l(x-q_l-\Delta_l)+\frac{3}{2}m_{l'}(x-q_{l'}-\Delta_{l'})\right], \tag{3.10}$$

$$\Delta_l=\frac{1}{3m_l}\ln\prod_{n\neq l}\left|\frac{m_l-m_n}{m_l+m_n}\right|.$$

The corresponding solution $v(t,x)$ of the KdV equation obtained from (3.9) by making $q_l(t)=q_l(0)+tp_l/m_l$ is called the N-soliton solution. In particular, the one-soliton solution is given by

$$s(t,x)=-\tfrac{9}{2}m^2\,\mathrm{sech}^2[\tfrac{3}{2}m(x-q(t))], \tag{3.11}$$

which represents a pulse of permanent shape whose center moves according to the free-particle trajectory $q(t)$. The most interesting property of the N-soliton solutions is that as $t\to\pm\infty$, they appear as a superposition[14] of N one-soliton solutions which emerge from the interaction with the same form and speed. The asymptotic trajectories $q_l(t)$ of the centers of these N one-soliton solutions as $t\to\pm\infty$ turn out to be

$$q_l^{\pm}(t) = q_l(t) + \delta_l^{\pm}, \tag{3.12}$$

where the shifts $\delta_l^{\pm}$ with respect to the free-particle trajectories $q_1(t)$ are

$$\delta_l^+ = -\delta_l^- = \frac{1}{3m_l} \times \left[\ln \prod_{n>l} \left| \frac{m_l - m_n}{m_l + m_n} \right| - \ln \prod_{n<l} \left| \frac{m_l - m_n}{m_l + m_n} \right| \right]. \tag{3.13}$$

It is worth noting that, due to the existence of these shifts, the motion of the asymptotic soliton components is of an interacting character. Thus it provides a picture of the dynamics of the KdV equation different from the one arising in the description through the free-particle variables (q_l, p_l).

C. Continuous degrees of freedom

According to (2.12b), the functions $q(k)$ and $p(k)$ which describe the continuous scattering data variables satisfy

$$q(k) \in \mathbb{R}(\text{mod } 2\pi), \quad p(k) \geqslant 0. \tag{3.14}$$

Let us define the complex-valued function

$$\phi(k) = (\tfrac{1}{2} k p(\tfrac{1}{2}k))^{1/2} \exp(iq(\tfrac{1}{2}k))$$
$$\text{for} \quad k \geqslant 0, \quad \phi(k) = \phi^*(-k) \quad \text{for} \quad k \leqslant 0. \tag{3.15}$$

Under ordinary conditions,[15] the function $\phi(k)$ is rapidly decreasing as $|k| \to \infty$. On the other hand, from the asymptotic behavior of $\ln|a(k)|^2$ as $k \to 0$, and since $|\phi(k)|^2 = (2\pi)^{-1} k^2 \ln|a(k/2)|^2$, it follows that $|(1/k)\phi(k)|^2$ is locally integrable around $k = 0$. All this implies that the function $\phi(k)/ik$ belongs to $L^2(\mathbb{R})$ and then it admits a Fourier transform

$$u(x) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{ikx} \frac{\phi(k)}{ik} dk. \tag{3.16}$$

Note that $u(x)$ is a real function whose derivative u_x is the Fourier transform of $\phi(k)$. In this way $u = u(x)$ provides an alternative description of the degrees of freedom associated with the continuous part of the scattering data variables. It is straightforward to rewrite the integral terms of the expressions (3.3) for the Galilean generators in terms of the new variable $u(x)$. One finds at once

$$M_c = \frac{1}{6} \int_0^{\infty} \frac{1}{k} p(k) dk = \frac{1}{6} \int_{-\infty}^{\infty} u^2 dx, \tag{3.17a}$$

$$P_c = -2 \int_0^{\infty} k p(k) dk = -\frac{1}{2} \int_{-\infty}^{\infty} u_x^2 dx, \tag{3.17b}$$

$$H_c = 8 \int_0^{\infty} k^3 p(k) dk = \frac{1}{2} \int_{-\infty}^{\infty} u_{xx}^2 dx, \tag{3.17c}$$

$$K_c = \frac{1}{12} \int_0^{\infty} \dot{q}(k) p(k) dk = -\frac{1}{6} \int_{-\infty}^{\infty} x u^2 dx. \tag{3.17d}$$

It is interesting to notice that in this representation, the functional $-K_c/M_c$ acquires the typical Galilean interpretation as the center of mass of the field $u(x)$. We may also write the continuous part of the symplectic structure Ω in terms of the new variable $u(x)$, and the result is

$$\Omega_c = \int_0^{\infty} (dp(k) \wedge dq(k))(\delta u_1, \delta u_2) dk = -\int_{-\infty}^{\infty} \delta u_1 \partial_x \delta u_2 \, dx. \tag{3.18}$$

From (3.17c) and (3.18) we have that the evolution law of the field $u(x)$ is given by the linear evolution equation

$$u_t = -u_{xxx}. \tag{3.19}$$

Therefore we see that by means of a Fourier transform of an appropriate combination of the continuous scattering data variables, the continuous component of the KdV flow reduces in such a way that the nonlinear term of the KdV equation drops out.

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APPENDIX

A proof of (2.29) for reflectionless potentials follows from the N-soliton formula[14]

$$v(x) = -2\partial_{xx} \ln \det(\mathbb{1} + C), \tag{A1}$$

$$C_{lm} = \frac{c_l c_m}{|k_l| + |k_m|} \exp[-(|k_l| + |k_m|)x], \tag{A2}$$

where k_l, denotes the N zeros of $a(k)$ and

$$c_l = |\dot{a}(k_l) b_l|^{-1/2}. \tag{A3}$$

By direct integration we have that

$$\int_{-\infty}^{\infty} x v(x) dx = 2 \lim_{x \to -\infty} [x \partial_x \ln \det(\mathbb{1} + C) - \ln \det(\mathbb{1} + C)]. \tag{A4}$$

Therefore we need only determine the asymptotic expression of $\det(\mathbb{1} + C)$ as $x \to -\infty$. We first note[14] that $\det(\mathbb{1} + C)$ is of the form

$$\det(\mathbb{1} + C) = 1 + \sum_l \alpha_l \exp(-\beta_l x), \tag{A5}$$

where the terms $\alpha_l \exp(-\beta_l x)$ are the principal minors of C of every order which have the same form as C itself. Indeed, from (A2) it follows that $\det C = \alpha_1 \exp(-\beta_1 x)$, where

$$\alpha_1 = \det(1/|k_l| + |k_m|) \prod_l c_l^2, \quad \beta_1 = \sum_l |k_l|. \tag{A6}$$

Clearly the term $\alpha_1 \exp(-\beta_1 x)$ in (A5) dominates as $x \to -\infty$. Hence by writing

$$\det(\mathbb{1} + C) = \alpha_1 e^{-\beta_1 x} \left(1 + \frac{1}{\alpha_1} e^{\beta_1 x} + \frac{1}{\alpha_1} \sum_{l \neq 1} \alpha_l e^{(\beta_1 - \beta_l)x} \right), \tag{A7}$$

it is evident that

$$\int_{-\infty}^{\infty} x v(x) dx = -2 \ln \alpha_1. \tag{A8}$$

Next let us consider α_1. Under the reflectionless condition, the function $a(k)$ is simply

$$a(k) = \prod_l \frac{k - k_l}{k + k_l}. \tag{A9}$$

Then from (A3) and (A9), we deduce

$$\prod_l c_l^2 = 2^{-N}\left(\prod_l |b_l\, k_l|^{-1}\right) \prod_{l<m} \left|\frac{k_l - k_m}{k_l + k_m}\right|^2. \tag{A10}$$

Therefore by using the identity

$$\det\left(\frac{1}{x_l + x_m}\right) = 2^{-N}\left(\prod_l x_l^{-1}\right) \prod_{l<m} \left(\frac{x_l - x_m}{x_l + x_m}\right)^2, \tag{A11}$$

it follows that

$$\alpha_1 = \prod_l \frac{1}{|b_l|} \tag{A12}$$

and, consequently,

$$\int_{-\infty}^{\infty} xv(x)dx = 2 \sum_l \ln |b_l|. \tag{A13}$$

This proves (2.29) for reflectionless potentials.

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Graded tensor calculus

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We develop a graded tensor calculus corresponding to arbitrary abelian groups of degrees and arbitrary commutation factors. The standard basic constructions and definitions, like tensor products, spaces of multilinear mappings, contractions, symmetrization, symmetric algebra, as well as the transpose, adjoint, and trace of a linear mapping, are generalized to the graded case and a multitude of canonical isomorphisms is presented. Moreover, the graded versions of the classical Lie algebras are introduced, and some of their basic properties are described.

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1. INTRODUCTION

The present work is the first in a series of papers in which we propose to investigate the invariants of Lie superalgebras[1,2] and, in particular, their Casimir elements. Our results should include (or, at least, be pertinent to) various topics in the representation theory of Lie superalgebras such as the classification of irreducible representations by means of the eigenvalues of Casimir operators, the study of tensor operators, the specification of states in a representation by means of chains of subalgebras, the breaking of supersymmetry, etc.

For obvious reasons we shall concentrate on the classical simple Lie superalgebras. Even for these we are going to meet a lot of complications and surprises. Let us recall that, in general, the finite-dimensional representations are not completely reducible and that certain "nontypical" irreducible representations are not completely specified by the eigenvalues of the Casimir operators.[3-5] Furthermore, we shall see that for spl(2,1) the algebra of Casimir elements, i.e., the center (in the graded sense) of the enveloping algebra, is not finitely generated. This is by no means special to spl(2,1), in fact, our subsequent investigations show that this phenomenon occurs for most of the general linear, special linear, and orthosymplectic Lie superalgebras.

In the present paper we are going to set up the formal foundation for our investigations by developing the graded tensor calculus. The reader may wonder whether anything new can be said in this field because such a calculus already seems to exist (for example, see Ref. 2). But there are certain aspects which to our opinion have not yet satisfactorily been treated. The most noteworthy topic is the contraction of tensors (see Sec. 11). Of course, partial results are known (the supertrace being a good example), but what seems to be missing is a systematic treatment which also includes the contraction with respect to *odd* bilinear forms. Furthermore, let us draw the reader's attention to Sec. 5, where the action of the symmetric group is discussed, to Sec. 8, which gives an intrinsic definition of the supertrace, to Secs. 7 and 9, where the supertranspose and the superadjoint of a linear mapping are introduced, and to Sec. 12 in which the supersymmetric algebra of a graded vector space is investigated. On the whole, the emphasis will be on the coherence and flexibility of the calculus. Thus we present a multitude of canonical homomorphisms and commutative diagrams (in particular, see Sec. 6).

In view of the formal character of the present work, the reader might anticipate that our results apply equally well to the so-called ϵ Lie algebras.[6] This is indeed the case, and we shall present them in this more general setting (part of our material has been obtained independently by Agrawala[7]).

Recall that the ϵ Lie algebras have been introduced into physics in Ref. 8, but they were known long ago in the mathematical literature.[9,10] (I am grateful to M. Duflo for drawing my attention to these latter references.) It is well known that the arguments leading to the classical Lie superalgebras immediately generalize to the ϵ Lie algebra case. The algebras analogous to the special linear, orthosymplectic, and P-type [that is, $b(n)$] Lie superalgebras are introduced in the Secs. 8 and 10. Also, we remark that our tensor calculus for graded modules over an ϵ Lie algebra L is just an elaboration and extension of the theory of graded algebras and modules as can be found in the mathematical literature.[11,12] This could be made evident by explicitly reducing the basic definitions on graded L-modules to those on graded $U(L)$-modules [with $U(L)$ the enveloping algebra of L]; for the Z_2-graded case this has been carried out in Ref. 2.

Note that, by restricting our attention to Lie superalgebras, we would save but a few lines. On the other hand, it is well known that most of the simple Lie superalgebras have a natural Z-gradation, and it may be quite useful (even in practical calculations) to take advantage of this finer structure. Let us stress, however, that we shall not hesitate to consider only Lie superalgebras whenever the more general case causes additional problems.

We close this introduction by collecting a few conventions. Throughout this work K will denote a commutative field of characteristic zero, Γ will stand for an abelian group, ϵ will be a commutation factor on Γ with values in K, and L will denote an ϵ Lie algebra (the definitions will be repeated in Sec. 2). The reader who is interested only in Lie superalgebras may set $\Gamma = Z_2$ and $\epsilon(\alpha, \beta) = (-1)^{\alpha\beta}$. All vector spaces and algebras are supposed to have K as their field of scalars. Let us stress that the algebras and vector spaces are not necessarily finite-dimensional unless otherwise stated. We recall that infinite-dimensional highest weight modules play a vital role in the theory of representations.

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2. SOME BASIC DEFINITIONS

A *vector space* V is said to be *Γ-graded* if we are given a family $(V_\gamma)_{\gamma\in\Gamma}$ of subspaces of V such that V is their direct sum,

$$V = \bigoplus_{\gamma\in\Gamma} V_\gamma . \qquad (2.1)$$

An *element* of V is said to be *homogeneous of degree* $\gamma\in\Gamma$ if it is an element of V_γ. Note that the degree of a nonzero homogeneous element is uniquely fixed, but that 0 is homogeneous of any degree. A *subspace* V' of V is said to be *graded* if

$$V' = \bigoplus_{\gamma\in\Gamma} (V'\cap V_\gamma) . \qquad (2.2)$$

If the base field K is considered as a graded vector space, it is always understood that the gradation of K is given by

$$K_0 = K ,$$
$$K_\gamma = \{0\} \quad \text{if } \gamma\in\Gamma - \{0\} . \qquad (2.3)$$

A. Convention

In the following we shall frequently be talking about homogeneous elements of graded vector spaces. To simplify the formulation, let us agree to denote the degree of any homogeneous element by the "corresponding" lower case Greek letter (in case the element we are talking about is equal to zero the Greek letter may be any element of Γ). Thus, if A, B', C_i,..., g, h,..., R, $\tilde{S}$, t,..., X, y, Z are some homogeneous elements, it is tacitly understood that they are homogeneous of degree α, β', γ_i,..., γ, η,..., ρ, $\tilde{\sigma}$, τ,..., ξ, η, ζ, respectively. Only occasionally (but, of course, in all cases where there could be any doubts) the degrees will be specified explicitly.

Now let V and W be two Γ-graded vector spaces. A *linear mapping* g: $V\to W$ is said to be *homogeneous of degree* γ if $g(x)$ is homogeneous of degree $\gamma + \xi$ whenever the element $x\in V$ is homogeneous of degree ξ. The vector space of all such mappings will be denoted by $\mathrm{Lgr}(V,W)_\gamma$; it is a subspace of $L(V,W)$, the vector space of all linear mappings of V into W. We define $\mathrm{Lgr}(V,W)$ to be the sum of these subspaces; obviously, this sum is direct,

$$\mathrm{Lgr}(V,W) = \bigoplus_{\gamma\in\Gamma} \mathrm{Lgr}(V,W)_\gamma . \qquad (2.4)$$

Thus $\mathrm{Lgr}(V,W)$ is a Γ-graded vector space [recall that in Ref. 6 the space $\mathrm{Lgr}(V,W)$ has been denoted by $\mathrm{Homgr}(V,W)$]. We remark that this space is equal to $L(V,W)$ if (for example) the homogeneous components of V and W are equal to $\{0\}$ for all but a finite number of degrees.

Let U, V, W be three Γ-graded vector spaces and let h: $U\to V$ and g: $V\to W$ be two linear mappings. If h is homogeneous of degree η and g is homogeneous of degree γ, then $g\circ h$ is homogeneous of degree $\gamma + \eta$.

An *algebra* S is called *Γ-graded* if its underlying vector space is Γ-graded,

$$S = \bigoplus_{\gamma\in\Gamma} S_\gamma , \qquad (2.5)$$

and if, furthermore,

$$S_\alpha S_\beta \subset S_{\alpha+\beta} \quad \text{for all } \alpha,\beta\in\Gamma . \qquad (2.6)$$

If S has a unit element e it follows that $e\in S_0$. A subalgebra or an ideal of S is said to be graded if it is graded as a subspace of S.

Let T be a second Γ-graded algebra. A mapping $S\to T$ is called a *homomorphism of Γ-graded algebras* if it is a homomorphism of the algebra S into the algebra T which is homogeneous of degree zero.

Suppose I is a graded two-sided ideal of S. There exists on S/I a unique Γ-gradation such that the canonical mapping $S\to S/I$ is homogeneous of degree zero. Endowed with this gradation, S/I is a Γ-graded algebra, and the canonical mapping $S\to S/I$ is a homomorphism of graded algebras.

Example 2.1: Let V be a Γ-graded vector space. The Γ-graded vector space $\mathrm{Lgr}(V,V)$, endowed with the usual multiplication (i.e., composition) of linear mappings is an associative Γ-graded algebra.

Definition 2.1: A *commutation factor* on Γ with values in K is a mapping

$$\epsilon\colon \Gamma\times\Gamma\to K \qquad (2.7a)$$

such that

$$\epsilon(\alpha,\beta)\epsilon(\beta,\alpha) = 1 , \qquad (2.7b)$$
$$\epsilon(\alpha,\beta+\gamma) = \epsilon(\alpha,\beta)\epsilon(\alpha,\gamma) , \qquad (2.7c)$$
$$\epsilon(\alpha+\beta,\gamma) = \epsilon(\alpha,\gamma)\epsilon(\beta,\gamma) \qquad (2.7d)$$

for all α, β,$\gamma\in\Gamma$.

It follows from the definition that $\gamma\to\epsilon(\gamma,\gamma)$ is a homomorphism of the group Γ into the multiplicative group $\{1,-1\}$. An element $\gamma\in\Gamma$ is called *even* or *odd* if $\epsilon(\gamma,\gamma)$ is equal to 1 or -1, respectively; an element x of a Γ-graded vector space $V = \oplus_{\gamma\in\Gamma} V_\gamma$ is said to be *even* or *odd* if x is an element of $\otimes_{\gamma\,\mathrm{even}} V_\gamma$ or $\otimes_{\gamma\,\mathrm{odd}} V_\gamma$, respectively.

Definition 2.2: Let ϵ be a commutation factor on Γ. A Γ-graded algebra

$$L = \bigoplus_{\gamma\in\Gamma} L_\gamma , \qquad (2.8)$$

whose product mapping is denoted by a pointed bracket $\langle\ ,\ \rangle$, is called an *ϵ Lie algebra* if the following identities are satisfied:

$$\langle A,B\rangle = -\epsilon(\alpha,\beta)\langle B,A\rangle , \quad \epsilon \text{ skew-symmetry} , \qquad (2.9)$$
$$\epsilon(\gamma,\alpha)\langle A,\langle B,C\rangle\rangle + \text{cyclic} = 0 , \quad \epsilon \text{ Jacobi identity} , \qquad (2.10)$$

for all homogeneous elements A,B,$C\in L$.

Example 2.2: Let S be an associative Γ-graded algebra. On the Γ-graded vector space S we define a new multiplication $\langle\ ,\ \rangle$, the *ϵ-commutator*, by the requirement that

$$\langle a,b\rangle = ab - \epsilon(\alpha,\beta)ba \qquad (2.11)$$

for all homogeneous elements a,$b\in S$. It is easy to see that the bracket $\langle\ ,\ \rangle$ turns S into an ϵ Lie algebra which is said to be associated with S and which will be denoted by $S(\epsilon)$.

For later reference let us also introduce the *ϵ-anticommutator* $\langle\ ,\ \rangle_+$ which is defined to be the unique bilinear mapping of $S\times S$ into S such that

$$\langle a,b\rangle_+ = ab + \epsilon(\alpha,\beta)ba \qquad (2.12)$$

for all homogeneous elements a,$b\in S$.

Example 2.3: Let V be a Γ-graded vector space. We know that $\mathrm{Lgr}(V,V)$ is an associative Γ-graded algebra (see Example 2.1). The ϵ Lie algebra which is associated with $\mathrm{Lgr}(V,V)$ is called the *general linear ϵ Lie algebra* of V and will be denoted by $\mathrm{gl}(V,\epsilon)$.

Example 2.4: Let T be a Γ-graded algebra. For any $\delta\in\Gamma$, let $D(T,\epsilon)_\delta$ denote the subspace of all elements $D\in\mathrm{gl}(V,\epsilon)_\delta$ such that

$$D(ab) = D(a)b + \epsilon(\delta,\alpha)aD(b) \tag{2.13}$$

for all homogeneous elements $a,b\in T$. It is easy to see that

$$D(T,\epsilon) = \bigoplus_{\delta\in\Gamma} D(T,\epsilon)_\delta \tag{2.14}$$

is a graded subalgebra of $\mathrm{gl}(T,\epsilon)$. The elements of $D(T,\epsilon)$ are called the *ϵ-derivations* of T.

If T is associative, the mapping $a\rightarrow\langle a,\cdot\rangle$ is a graded algebra homomorphism of $T(\epsilon)$ into $D(T,\epsilon)$ (see Example 2.2). For any ϵ Lie algebra L, the mapping $A\rightarrow\langle A,\cdot\rangle$ is a graded algebra homomorphism of L into $D(L,\epsilon)$.

Definition 2.3: Let L be an ϵ Lie algebra. A *graded representation* of L in a Γ-graded vector space V is a homomorphism ρ: $L\rightarrow\mathrm{gl}(V,\epsilon)$ of Γ-graded algebras (this implies that ρ is homogeneous of degree zero). A Γ-graded vector space V which is endowed with a graded representation of L is called a *graded L-module.*

For any graded L-module V, the representative of an element $A\in L$ will frequently be denoted by A_V. If x is an element of V, we shall sometimes even write Ax instead of $A_V x$.

Let V and W be two graded L-modules. A linear mapping g: $V\rightarrow W$ which is homogeneous of degree zero and which satisfies

$$A_W \circ g = g\circ A_V \quad \text{for all } A\in L \tag{2.15}$$

is called a *homomorphism of graded L-modules.*

Graded submodules, graded quotient modules (with respect to graded submodules), and direct sums of graded L-modules are defined in the obvious way.

Example 2.5: The mapping $A\rightarrow\mathrm{ad}\,A = \langle A,\cdot\rangle$ is a graded representation of L in the Γ-graded vector space L (see Example 2.4); it is called the *adjoint representation* of L and the Γ-graded vector space L, endowed with this representation, is called the *adjoint L-module*. If L is considered as a graded L-module it is always understood that L is endowed with the adjoint representation.

Example 2.6: On any Γ-graded vector space V there is the so-called *trivial L-module structure*, defined by $A_V = 0$ for all $A\in L$. If K is considered as a graded L-module, it is always understood that its L-module structure is trivial, unless otherwise stated.

Example 2.7: Let V be a Γ-graded vector space. For any $\alpha\in\Gamma$, we construct a new Γ-graded vector space V^α by requiring that V and V^α coincide as (nongraded) vector spaces but that $V^\alpha_\gamma = V_{\alpha+\gamma}$ for all $\gamma\in\Gamma$. We say that V^α is obtained from V by a *shift of the Γ-gradation*. Obviously, $\mathrm{Lgr}(V,V)$ and $\mathrm{Lgr}(V^\alpha,V^\alpha)$ coincide as Γ-graded algebras; hence $\mathrm{gl}(V,\epsilon)$ and $\mathrm{gl}(V^\alpha,\epsilon)$ do likewise. It follows that any graded representation of L in V is also a graded representation of L in V^α. According to our conventions, these two representations are not isomorphic, in general.

Definition 2.4: Let V be a graded L-module. An element $x\in V$ is said to be *L-invariant* (or, more simply, invariant) if

$$A_V x = 0 \quad \text{for all } A\in L. \tag{2.16}$$

Obviously, the set of all L-invariant elements of V is a graded subspace of V, i.e., an element of V is L-invariant if and only if all its homogeneous components are.

Conversely, let x be a fixed *homogeneous* element of a graded L-module V. An element $A\in L$ is said to leave x invariant if $A_V x = 0$. The set of all such elements A is a graded subalgebra of L.

3. TENSOR PRODUCTS OF GRADED L-MODULES

Let V_i, $1\leqslant i\leqslant n$, be Γ-graded vector spaces. For any $\gamma\in\Gamma$, we denote by $(V_1\otimes\cdots\otimes V_n)_\gamma$ the subspace of $V_1\otimes\cdots\otimes V_n$, which is generated by the tensors of the form $x_1\otimes\cdots\otimes x_n$, where the elements $x_i\in V_i$ are homogeneous of degree ξ_i, with $\xi_1+\cdots+\xi_n=\gamma$. It is well known that

$$V_1\otimes\cdots\otimes V_n = \bigoplus_{\gamma\in\Gamma}(V_1\otimes\cdots\otimes V_n)_\gamma, \tag{3.1}$$

i.e., the subspaces $(V_1\otimes\cdots\otimes V_n)_\gamma$ form a Γ-gradation of $V_1\otimes\cdots\otimes V_n$. In the following, a tensor product of Γ-graded vector spaces will always be endowed with this Γ-gradation. Occasionally, it is advantageous to set the empty tensor product equal to K (case $n=0$).

Now let W_i, $1\leqslant i\leqslant n$, be a second family of n Γ-graded vector spaces. Suppose we are given, for every $i\in\{1,\dots,n\}$, a linear mapping g_i: $V_i\rightarrow W_i$ which is homogeneous of degree γ_i. Then there exists a unique linear mapping

$$g_1\,\overline{\otimes}\cdots\overline{\otimes}\,g_n:\; V_1\otimes\cdots\otimes V_n\rightarrow W_1\otimes\cdots\otimes W_n \tag{3.2a}$$

such that

$$(g_1\,\overline{\otimes}\cdots\overline{\otimes}\,g_n)(x_1\otimes\cdots\otimes x_n) = \prod_{i>j}\epsilon(\gamma_i,\xi_j)\,g_1(x_1)\otimes\cdots\otimes g_n(x_n) \tag{3.2b}$$

for all homogeneous elements $x_i\in V_i$. Obviously, $g_1\,\overline{\otimes}\cdots\overline{\otimes}\,g_n$ is homogeneous of degree $\gamma=\gamma_1+\cdots+\gamma_n$, and the mapping

$$(g_1,\dots,g_n)\rightarrow g_1\,\overline{\otimes}\cdots\overline{\otimes}\,g_n \tag{3.3}$$

of $\Pi\,\mathrm{Lgr}(V_i,W_i)_{\gamma_i}$ into $\mathrm{Lgr}(\otimes V_i,\otimes W_i)_\gamma$ is n-linear. It follows that there exists a unique linear mapping

$$\pi:\; \bigotimes_{i=1}^{n}\mathrm{Lgr}(V_i,W_i)\rightarrow\mathrm{Lgr}\Big(\bigotimes_{i=1}^{n}V_i,\;\bigotimes_{i=1}^{n}W_i\Big) \tag{3.4a}$$

such that

$$\pi(g_1\otimes\cdots\otimes g_n) = g_1\,\overline{\otimes}\cdots\overline{\otimes}\,g_n \tag{3.4b}$$

for all homogeneous linear mappings $g_i\in\mathrm{Lgr}(V_i,W_i)$. The mapping π is *homogeneous of degree zero* and *injective*; it is even bijective if the vector spaces V_i are all finite-dimensional. In the following, the mapping $\pi(g_1\otimes\cdots\otimes g_n)$ will be denoted by $g_1\,\overline{\otimes}\cdots\overline{\otimes}\,g_n$ even if the g_i are not necessarily homogeneous.

Let U_i, $1\leqslant i\leqslant n$, be a third family of n Γ-graded vector spaces. If we are given, for every $i\in\{1,\dots,n\}$, the linear mappings h_i: $U_i\rightarrow V_i$ and g_i: $V_i\rightarrow W_i$, which are homogeneous of degree η_i and γ_i, respectively, then

$$(g_1 \overline{\otimes} \cdots \overline{\otimes} g_n) \circ (h_1 \overline{\otimes} \cdots \overline{\otimes} h_n)$$
$$= \prod_{i>j} \epsilon(\gamma_i, \eta_j)\, (g_1 \circ h_1) \overline{\otimes} \cdots \overline{\otimes} (g_n \circ h_n) . \tag{3.5}$$

Now assume that L_i is an ϵ Lie algebra and that ρ_i is a graded representation of L_i in V_i, for all $i \in \{1,...,n\}$. The Cartesian product $L_1 \times \cdots \times L_n$ is an ϵ Lie algebra in the obvious sense, and the mapping

$$(A_1,...,A_n) \mapsto \sum_{i=1}^{n} \mathrm{id}\, \overline{\otimes} \cdots \overline{\otimes}\, \rho_i(A_i) \overline{\otimes} \cdots \overline{\otimes}\, \mathrm{id} , \tag{3.6}$$

with $A_i \in L_i$, is a graded representation of $L_1 \times \cdots \times L_n$ in $V_1 \otimes \cdots \otimes V_n$.

Suppose next that the L_i are all equal to one fixed ϵ Lie algebra L. The diagonal mapping $A \to (A,...,A)$ is a graded algebra homomorphism of L into L^n. Consequently, the equation

$$\rho(A) = \sum_{i=1}^{n} \mathrm{id}\, \overline{\otimes} \cdots \overline{\otimes}\, \rho_i(A) \overline{\otimes} \cdots \overline{\otimes}\, \mathrm{id} , \tag{3.7}$$

with $A \in L$, defines a graded representation ρ of L in $V_1 \otimes \cdots \otimes V_n$. We call ρ the *graded tensor product of the representations* ρ_i and $V_1 \otimes \cdots \otimes V_n$, endowed with this representation, the *graded tensor product of the L-modules* V_i.

It is easy to see that the graded tensor product of graded L-modules is *associative* in the obvious sense. The question of commutativity is somewhat more subtle and will be discussed in Sec. 5. Let us also remark that, for any graded L-module V, the tensor products $K \otimes V$ and $V \otimes K$ are canonically isomorphic to V (provided that K is endowed with the trivial L-module structure).

To give an application, let V be a graded L-module and let $T(V) = \oplus_{n \in Z} T_n(V)$ be the tensor algebra of V. We recall that $T(V)$ is a $Z \times \Gamma$-graded algebra with $T_n(V) = \{0\}$ if $n \leqslant -1$, $T_0(V) = K$, and $T_n(V) = V \otimes \cdots \otimes V$ (n factors) if $n \geqslant 1$. By the above, all the $T_n(V)$, $n \geqslant 1$, are graded L-modules. We introduce on $T_0(V)$ the trivial L-module structure and consider $T(V)$ as the direct sum of the graded L-modules $T_n(V)$, $n \geqslant 0$. It is easy to see that, for any $A \in L$, the representative A_T of A with respect to this structure is the unique ϵ-derivation of the algebra $T(V)$ which extends the mapping A_V of $T_1(V) = V$ into itself.

4. MULTILINEAR MAPPINGS BETWEEN GRADED L-MODULES

Let $V_1,...,V_n, W$ be Γ-graded vector spaces. An *n-linear mapping* g: $V_1 \times \cdots \times V_n \to W$ is said to be *homogeneous of degree* γ if $g(x_1,...,x_n)$ is homogeneous of degree $\gamma + \xi_1 + \cdots + \xi_n$ whenever the elements $x_i \in V_i$ are homogeneous of degree ξ_i. The vector space of all such mappings will be denoted by $\mathrm{Lgr}_n(V_1,...,V_n;W)_\gamma$, it is a subspace of $L_n(V_1,...,V_n;W)$, the vector space of all n-linear mappings of $V_1 \times \cdots \times V_n$ into W. We define $\mathrm{Lgr}_n(V_1,...,V_n;W)$ to be the sum of these subspaces; obviously, this sum is direct,

$$\mathrm{Lgr}_n(V_1,...,V_n;W) = \bigoplus_{\gamma \in \Gamma} \mathrm{Lgr}_n(V_1,...,V_n;W)_\gamma . \tag{4.1}$$

Thus $\mathrm{Lgr}_n(V_1,...,V_n;W)$ is a Γ-graded vector space. We remark that this space is equal to $L_n(V_1,...,V_n;W)$ if (for example) the homogeneous components of $V_1,...,V_n, W$ are equal to $\{0\}$ for all but a finite number of degrees. Note also that $\mathrm{Lgr}_1(V_1;W) = \mathrm{Lgr}(V_1, W)$. Occasionally, it is advantageous to set $\mathrm{Lgr}_0(\ ;W) = W$.

Suppose now that $\rho_1,..., \rho_n, \rho_0$ are graded representations of an ϵ Lie algebra L in the Γ-graded vector spaces $V_1,...,V_n, W$, respectively. Then there is a unique graded representation σ of L in $\mathrm{Lgr}_n(V_1,...,V_n;W)$ such that

$$(\sigma(A)g)(x_1,...,x_n) = \rho_0(A)g(x_1,...,x_n) - \sum_{i=1}^{n} \epsilon(\alpha, \gamma + \sum_{j<i} \xi_j)$$
$$\times g(x_1,..., \rho_i(A)x_i,...,x_n) \tag{4.2}$$

for all homogeneous elements $A \in L$, $g \in \mathrm{Lgr}_n(V_1,...,V_n;W)$, and $x_i \in V_i$.

The case $n = 1$ is particularly important; we reformulate it as follows. If V and W are graded L-modules, there exists on $\mathrm{Lgr}(V, W)$ a unique graded L-module structure such that

$$Ag = A_W \circ g - \epsilon(\alpha,\gamma) g \circ A_V \tag{4.3}$$

for all homogeneous elements $A \in L$ and $g \in \mathrm{Lgr}(V, W)$.

As a special case let us assume that $W = K$ (endowed with the trivial L-module structure). For any Γ-graded vector space V, the space

$$V^{*\mathrm{gr}} = \mathrm{Lgr}(V,K) \tag{4.4}$$

is called the *graded dual* of V. Consequently, if V is a graded L-module, there exists on $V^{*\mathrm{gr}}$ a unique graded L-module structure such that

$$A_{V^*} g = -\epsilon(\alpha,\gamma) g \circ A_V \tag{4.5}$$

for all homogeneous elements $A \in L$ and $g \in V^{*\mathrm{gr}}$. Endowed with this structure, $V^{*\mathrm{gr}}$ will be called the *graded dual* of the L-module V or the L-module *contragredient* to V.

Example 4.1: The graded dual of the adjoint L-module will be called the *coadjoint L-module*.

Resuming our general discussion, we shall now show that, by use of Sec. 3, the general definition (4.2) can be reduced to the case $n = 1$. In fact, let $V_1,...,V_n, W$ be Γ-graded vector spaces. By definition of the tensor product $V_1 \otimes \cdots \otimes V_n$, there exists a canonical isomorphism of $L_n(V_1,...,V_n;W)$ onto $L(V_1 \otimes \cdots \otimes V_n, W)$ which maps any n-linear mapping

$$g\colon\ V_1 \times \cdots \times V_n \to W \tag{4.6a}$$

onto the linear mapping

$$\tilde{g}\colon\ V_1 \otimes \cdots \otimes V_n \to W, \tag{4.6b}$$

which satisfies

$$\tilde{g}(x_1 \otimes \cdots \otimes x_n) = g(x_1,...,x_n) \tag{4.6c}$$

for all $x_i \in V_i$. Obviously, g is homogeneous of degree γ if and only if $\tilde{g}$ is homogeneous of degree γ. Consequently, the mapping

$$\mu\colon\ \mathrm{Lgr}_n(V_1,...,V_n;W) \mapsto \mathrm{Lgr}(V_1 \otimes \cdots \otimes V_n, W) , \tag{4.7a}$$

with

$$\mu(g) = \tilde{g} \quad \text{for all } g \in \mathrm{Lgr}_n(V_1,...,V_n;W) , \tag{4.7b}$$

is a well-defined isomorphism of Γ-graded vector spaces. If we now assume that $V_1,...,V_n, W$ are graded L-modules, it is easy to see that μ is even a canonical *isomorphism of graded L-modules*.

Once the spaces $\mathrm{Lgr}_n(V_1,\dots,V_n;W)$ are endowed with a graded L-module structure, we can talk about invariant multilinear mappings. The general definition can be read off from Eq. (4.2); we do not write out the details. However, let us remark that if the mapping $g\in\mathrm{Lgr}_n(V_1,\dots,V_n;W)$ and the elements $x_i\in V_i$; $1\leqslant i\leqslant n$, are L-invariant, then $g(x_1,\dots,x_n)$ is L-invariant as well.

Example 4.2: Let V and W be two graded L-modules. A homogeneous linear mapping g: $V\to W$ is L-invariant if and only if

$$A_W\circ g=\epsilon(\alpha,\gamma)g\circ A_V \tag{4.8}$$

for all homogeneous elements $A\in L$. In particular, the homomorphisms of graded L-modules are just the linear mappings which are homogeneous of degree zero and L-invariant.

If the linear mapping g: $V\to W$ is injective, homogeneous, and L-invariant, then an element $x\in V$ is L-invariant if and only if $g(x)$ is L-invariant.

Example 4.3: For any three graded L-modules U, V, W, the bilinear mapping of $\mathrm{Lgr}(V,W)\times\mathrm{Lgr}(U,V)$ into $\mathrm{Lgr}(U,W)$, which associates with any pair (g,h) of mappings $g\in\mathrm{Lgr}(V,W)$ and $h\in\mathrm{Lgr}(U,V)$ the composed mapping $g\circ h$, is homogeneous of degree zero and L-invariant. In particular, if $g\in\mathrm{Lgr}(V,W)$ and $h\in\mathrm{Lgr}(U,V)$ are L-invariant, then so is $g\circ h$.

Example 4.4: Let T be a Γ-graded algebra. If T is endowed with its natural $\mathrm{gl}(T,\epsilon)$-module structure, the ϵ-derivations of T (see Example 2.4) are just the elements $D\in\mathrm{gl}(T,\epsilon)$ that leave the multiplication mapping $T\times T\to T$ invariant.

Example 4.5: Let V_i, $1\leqslant i\leqslant n$, be graded L-modules and let ρ_i: $L\to\mathrm{gl}(V_i,\epsilon)$ denote the corresponding graded representations. An n-linear form $g\in\mathrm{Lgr}_n(V_1,\dots,V_n;K)$ is L-invariant if and only if

$$\sum_{i=1}^{n}\epsilon\Big(\alpha,\sum_{j<i}\xi_j\Big)g(x_1,\dots,\rho_i(A)x_i,\dots,x_n)=0 \tag{4.9}$$

for all homogeneous elements $A\in L$ and $x_i\in V_i$.

Example 4.6: For any graded L-module V, the canonical bilinear form $V^{*\mathrm{gr}}\times V\to K$ is L-invariant. [Recall that, for any $x'\in V^{*\mathrm{gr}}$ and all $x\in V$, this form maps (x',x) onto $x'(x)$.]

5. ACTION OF THE SYMMETRIC GROUP

It is evident from the definition that in general the tensor product of graded L-modules is not commutative in the usual sense. Nevertheless, there exists a natural notion of ϵ-symmetry which perfectly serves to cure this defect.

For any integer $n\geqslant 1$ and any permutation π of $\{1,\dots,n\}$, we define

$$I(\pi)=\{(i,j)\,|\,1\leqslant i<j\leqslant n,\ \pi(i)>\pi(j)\}\ . \tag{5.1}$$

Now let V_i, $1\leqslant i\leqslant n$, be graded L-modules and let π be a permutation of $\{1,\dots,n\}$. There exists a unique linear mapping

$$S_\pi:\ V_1\otimes\cdots\otimes V_n\to V_{\pi^{-1}(1)}\otimes\cdots\otimes V_{\pi^{-1}(n)} \tag{5.2a}$$

such that

$$S_\pi(x_1\otimes\cdots\otimes x_n)=\prod_{(i,j)\in I(\pi)}\epsilon(\xi_i,\xi_j)\,x_{\pi^{-1}(1)}\otimes\cdots\otimes x_{\pi^{-1}(n)} \tag{5.2b}$$

for all homogeneous elements $x_i\in V_i$, $1\leqslant i\leqslant n$. It is easy to check that S_π is a canonical *isomorphism* of graded L-modules which is said to be associated with π.

If ρ is a second permutation of $\{1,\dots,n\}$ and if S_ρ^π is the isomorphism of $V_{\pi^{-1}(1)}\otimes\cdots\otimes V_{\pi^{-1}(n)}$ onto $V_{\pi^{-1}\rho^{-1}(1)}\otimes\cdots\otimes V_{\pi^{-1}\rho^{-1}(n)}$ associated with ρ, then

$$S_{\rho\pi}=S_\rho^\pi\circ S_\pi\ . \tag{5.3}$$

The discussion simplifies if the V_i are all equal to a fixed graded L-module V. In that case Eq. (5.3) says that $\pi\to S_\pi$ is a *representation* of the symmetric group $\mathfrak{S}_n$ by *automorphisms* of the graded L-module $T_n(V)=V\otimes\cdots\otimes V$.

Let V_i', $1\leqslant i\leqslant n$, be a second family of n graded L-modules. Suppose we are given, for every $i\in\{1,\dots,n\}$, a homogeneous linear mapping g_i: $V_i\to V_i'$ of degree γ_i. If S_π' is the isomorphism of $V_1'\otimes\cdots\otimes V_n'$ onto $V'_{\pi^{-1}(1)}\otimes\cdots\otimes V'_{\pi^{-1}(n)}$ associated with π, we have

$$S_\pi'\circ(g_1\bar{\otimes}\cdots\bar{\otimes}g_n)$$

$$=\prod_{(i,j)\in I(\pi)}\epsilon(\gamma_i,\gamma_j)\,(g_{\pi^{-1}(1)}\bar{\otimes}\cdots\bar{\otimes}g_{\pi^{-1}(n)})\circ S_\pi\ . \tag{5.4}$$

Example 5.1: For any two graded L-modules U and V there is a unique graded L-module isomorphism

$$s:\ U\otimes V\to V\otimes U \tag{5.5a}$$

such that

$$s(x\otimes y)=\epsilon(\xi,\eta)y\otimes x \tag{5.5b}$$

for all homogeneous elements $x\in U$ and $y\in V$. We call s the ϵ-symmetry of $U\otimes V$ onto $V\otimes U$.

The symmetry transformations S_π can easily be transcribed into symmetry transformations for modules of multilinear mappings. Thus let W be one more graded L-module. Evidently, the mapping of $\mathrm{Lgr}(V_{\pi(1)}\otimes\cdots\otimes V_{\pi(n)},W)$ into $\mathrm{Lgr}(V_1\otimes\cdots\otimes V_n,W)$ defined by $g\to g\circ S_{\pi^{-1}}$ is an isomorphism of graded L-modules. In view of the isomorphism (4.7) this shows that the mapping

$$\check{S}_\pi:\ \mathrm{Lgr}_n(V_{\pi(1)},\dots,V_{\pi(n)};W)\to\mathrm{Lgr}_n(V_1,\dots,V_n;W) \tag{5.6a}$$

defined by

$$(\check{S}_\pi h)(x_1,\dots,x_n)=\prod_{(i,j)\in I(\pi^{-1})}\epsilon(\xi_i,\xi_j)\,h(x_{\pi(1)},\dots,x_{\pi(n)}) \tag{5.6b}$$

for all homogeneous elements $x_i\in V_i$, $1\leqslant i\leqslant n$, is a canonical *isomorphism* of graded L-modules.

If ρ is a second permutation of $\{1,\dots,n\}$ and if $\check{S}_\pi^\rho$ is derived from $g\to g\circ S_{\pi^{-1}}^{\rho^{-1}}$ just as $\check{S}_\pi$ has been derived from $g\to g\circ S_{\pi^{-1}}$, then

$$\check{S}_{\rho\pi}=\check{S}_\rho\circ\check{S}_\pi^\rho\ . \tag{5.7}$$

Once again the discussion simplifies if $V_i=V$, $1\leqslant i\leqslant n$, with a fixed graded L-module V. In that case Eq. (5.7) says that $\pi\to\check{S}_\pi$ is a *representation* of the symmetric group $\mathfrak{S}_n$ by *automorphisms* of the graded L-module $\mathrm{Lgr}_n(V,\dots,V;W)$.

Example 5.2: For any three graded L-modules U, V, W there is a unique graded L-module isomorphism

$$s:\ \mathrm{Lgr}_2(V,U;W)\to\mathrm{Lgr}_2(U,V;W) \tag{5.8a}$$

such that

$$(sb)(x,y) = \epsilon(\xi,\eta)b(y,x) \tag{5.8b}$$

for all $b \in \mathrm{Lgr}_2(V,U;W)$ and all homogeneous elements $x \in U$ and $y \in V$. We call s the *ϵ-symmetry* of $\mathrm{Lgr}_2(V,U;W)$ onto $\mathrm{Lgr}_2(U,V;W)$.

We close this section by a few comments on the special case where $V_i = V$, $1 \leqslant i \leqslant n$, with a fixed graded L-module V. In that case we have the representations $\pi \to S_\pi$ and $\pi \to \check{S}_\pi$ of the symmetric group $\mathfrak{S}_n$ by automorphisms of the graded L-modules $T_n(V)$ and $\mathrm{Lgr}_n(V,...,V;W)$, respectively. Consequently, the standard representation theory of the symmetric group can be applied. In particular, we can decompose $T_n(V)$ and $\mathrm{Lgr}_n(V,...,V;W)$ into the direct sum of graded submodules corresponding to the various symmetry types. We do not want to enter these questions here but rather refer the reader to Refs. 13 and 14, where some more details are given. However, we shall occasionally use concepts such as ϵ-symmetry, ϵ-skew-symmetry, ϵ-symmetrization,... of tensors and multilinear mappings, which all have an obvious meaning. For example, an n-linear mapping $h \in \mathrm{Lgr}_n(V,...,V;W)$ is called ϵ-symmetric or ϵ-skew-symmetric if $\check{S}_\pi h = h$ or $\check{S}_\pi h = \mathrm{sgn}(\pi)h$, respectively, for all permutations $\pi \in \mathfrak{S}_n$.

6. CANONICAL HOMOMORPHISMS

As is well known, there exist several canonical homomorphisms between the tensor products of vector spaces and the spaces of multilinear mappings. In the present section we shall see that all these homomorphisms can be generalized to the graded case, provided some care is exercised with regard to the ordering of the various terms.

The reader will notice that the canonical homomorphisms to be described below are defined without taking recourse to any L-module structure, i.e., they make sense for Γ-graded vector spaces. Nevertheless, our main objective is to point out that these mappings are compatible with the graded L-module structures as well. Thus we shall formulate our results in this latter context; the case of Γ-graded vector spaces can then be obtained by simply setting $L = \{0\}$.

In the following it is always understood that all tensor products and all modules of multilinear mappings are endowed with the structure of a graded module over an ϵ Lie algebra according to the rules of Secs. 3 and 4.

(A) For all graded L-modules $V_1,...,V_n,W$ there exists a canonical *isomorphism* μ of $\mathrm{Lgr}_n(V_1,...,V_n;W)$ onto $\mathrm{Lgr}(V_1 \otimes \cdots \otimes V_n, W)$, which has already been discussed in Sec. 4 [see Eqs. (4.6) and (4.7)].

(B) For all $i \in \{1,...,n\}$, let L_i be an ϵ Lie algebra and let V_i and W_i be two graded L_i-modules. From Secs. 3 and 4 [in particular, see (3.6)] we infer that both $\otimes_{i=1}^n \mathrm{Lgr}(V_i,W_i)$ and $\mathrm{Lgr}(\otimes_{i=1}^n V_i, \otimes_{i=1}^n W_i)$ are endowed with a structure of a graded $\Pi_{i=1}^n L_i$-module. With respect to these structures, the mapping π of Eq. (3.4) is a canonical *injective homomorphism* of graded $\Pi_{i=1}^n L_i$-modules.

(C) Consider three graded L-modules, U, V, W. The linear mapping

$$\lambda_1\colon \mathrm{Lgr}(U, \mathrm{Lgr}(V,W)) \to \mathrm{Lgr}_2(U,V;W) \tag{6.1a}$$

defined by

$$(\lambda_1(g))(x,y) = (g(x))(y) \tag{6.1b}$$

for all $g \in \mathrm{Lgr}(U, \mathrm{Lgr}(V,W))$, $x \in U$, $y \in V$, is a canonical *isomorphism* of graded L-modules. This implies (see Example 5.2) that the mapping

$$\lambda_2\colon \mathrm{Lgr}(V, \mathrm{Lgr}(U,W)) \to \mathrm{Lgr}_2(U,V;W) \tag{6.2a}$$

defined by

$$(\lambda_2(g))(x,y) = \epsilon(\xi,\eta)(g(y))(x) \tag{6.2b}$$

for all $g \in \mathrm{Lgr}(V, \mathrm{Lgr}(U,W))$ and all homogeneous elements $x \in U$, $y \in V$, is a canonical *isomorphism* of graded L-modules as well.

In view of (A) we conclude that the graded L-modules $\mathrm{Lgr}(U, \mathrm{Lgr}(V,W))$, $\mathrm{Lgr}_2(U,V;W)$, $\mathrm{Lgr}(U \otimes V, W)$, and those with U and V interchanged, are all canonically isomorphic. To underline the relevance of these modules, let us remark that the invariant elements of $\mathrm{Lgr}(U, \mathrm{Lgr}(V,V))$ are just the *tensor operators* acting on V and transforming according to the representation in U.

Consider next the special case $W = K$. Let b be a homogeneous bilinear form on $U \times V$, of degree β, and let $g_1 \in \mathrm{Lgr}(U, V^{*\mathrm{gr}})$ and $g_2 \in \mathrm{Lgr}(V, U^{*\mathrm{gr}})$ be the linear mappings which correspond to b under the isomorphisms λ_1 and λ_2, respectively. We know that g_1 and g_2 are homogeneous of degree β, and if one of the mappings b, g_1, g_2 is L-invariant, so are the other two. Finally, b is nondegenerate if and only if g_1 and g_2 are injective.

As an example, let b be the canonical bilinear form on $V^{*\mathrm{gr}} \times V$. Then g_1 is the identity of $V^{*\mathrm{gr}}$ and g_2 is equal to the linear mapping

$$\nu\colon V \to (V^{*\mathrm{gr}})^{*\mathrm{gr}} \tag{6.3a}$$

defined by

$$(\nu(x))(x') = \epsilon(\xi,\xi')x'(x) \tag{6.3b}$$

for all homogeneous elements $x \in V$ and $x' \in V^{*\mathrm{gr}}$. According to the general remarks above, ν is a canonical *injective homomorphism* of graded L-modules. Note that $\nu(x)$ is equal to $\epsilon(\xi,\xi)$ times the usual (nongraded) canonical image of x in $(V^{*\mathrm{gr}})^{*\mathrm{gr}}$.

Returning to the general discussion, we shall now assume that U and V are finite-dimensional and that b is nondegenerate. Then g_1 and g_2 are bijective. Let $\tilde{b}$ be the linear form on $U \otimes V$ associated with b, and let $\check{b}$ denote the bilinear form on $V^{*\mathrm{gr}} \times U^{*\mathrm{gr}}$ associated with $\tilde{b} \circ (g_1^{-1} \overline{\otimes} g_2^{-1})$. It is easy to see that

$$\check{b}(g_1(x), g_2(y)) = \epsilon(\beta + \xi, \beta)b(x,y) \tag{6.4}$$

for all homogeneous elements $x \in U$ and $y \in V$. The bilinear form $\check{b}$ is homogeneous of degree $-\beta$ and nondegenerate; furthermore, our definition shows that if b is L-invariant, then so is $\check{b}$. We call $\check{b}$ the bilinear form *ϵ-inverse* to b.

Remark: We could equally well define the ϵ-inverse of b to be the bilinear form associated with $\tilde{b} \circ (g_1 \overline{\otimes} g_2)^{-1}$. This form is equal to $\epsilon(\beta,\beta)\check{b}$; thus the formula analogous to (6.4) is a little simpler. At present, I do not see any reason to prefer one of these definitions to the other.

(D) Let $V_1,...,V_n,W$ be graded L-modules. Then there exists a unique linear mapping

$$\omega:\ W\otimes V_n^{*\mathrm{gr}}\otimes\cdots\otimes V_1^{*\mathrm{gr}}\to \mathrm{Lgr}_n(V_1,\ldots,V_n;W) \tag{6.5a}$$

such that

$$(\omega(y\otimes x_n'\otimes\cdots\otimes x_1'))(x_1,\ldots,x_n)=\prod_{i=1}^n x_i'(x_i)\,y \tag{6.5b}$$

for all $y\in W$, $x_i'\in V_i^{*\mathrm{gr}}$, and $x_i\in V_i$. This mapping is, in fact, a canonical *injective homomorphism* of graded L-modules; it is bijective if the spaces V_i are finite-dimensional. (Note the special ordering of the modules: It avoids additional ϵ factors.)

The following two special cases are particularly important. For any two graded L-modules V and W there exists a unique linear mapping

$$\omega:\ W\otimes V^{*\mathrm{gr}}\to \mathrm{Lgr}(V,W) \tag{6.6a}$$

such that

$$(\omega(y\otimes x'))(x)=x'(x)\,y \tag{6.6b}$$

for all $y\in W$, $x'\in V^{*\mathrm{gr}}$, $x\in V$. This mapping is a canonical injective graded L-module homomorphism; it is bijective if V is finite-dimensional.

To obtain the second special case, we note that the homomorphism (6.5) can be composed with the isomorphism μ mentioned in (A). Choosing $W=K$ then yields a canonical injective L-module homomorphism of $V_n^{*\mathrm{gr}}\otimes\cdots\otimes V_1^{*\mathrm{gr}}$ into $(V_1\otimes\cdots\otimes V_n)^{*\mathrm{gr}}$ which is bijective if all the V_i are finite-dimensional.

Remark: At this point we would like to draw the reader's attention to a minor complication in connection with (6.5). For simplicity let us assume that $W=K$. If π is a permutation of $\{1,\ldots,n\}$, we have the canonical homomorphisms

$$\omega:\ V_n^{*\mathrm{gr}}\otimes\cdots\otimes V_1^{*\mathrm{gr}}\to \mathrm{Lgr}_n(V_1,\ldots,V_n;K)\,, \tag{6.7}$$

$$\omega':\ V_{\pi(n)}^{*\mathrm{gr}}\otimes\cdots\otimes V_{\pi(1)}^{*\mathrm{gr}}\to \mathrm{Lgr}_n(V_{\pi(1)},\ldots,V_{\pi(n)};K)\,. \tag{6.8}$$

The modules on the right are related through the isomorphism $\check{S}_\pi$ [see Eq. (5.6)]. To discuss the left-hand sides, let us define a permutation σ of $\{1,\ldots,n\}$ by

$$\sigma(r)=n+1-r \quad \text{for } 1\leqslant r\leqslant n\,. \tag{6.9}$$

If $S_{\sigma^{-1}\pi^{-1}\sigma}$ is the isomorphism of $V_{\sigma(1)}^{*\mathrm{gr}}\otimes\cdots\otimes V_{\sigma(n)}^{*\mathrm{gr}}$ onto $V_{\pi\sigma(1)}^{*\mathrm{gr}}\otimes\cdots\otimes V_{\pi\sigma(n)}^{*\mathrm{gr}}$ associated with $\sigma^{-1}\pi^{-1}\sigma$ [see Eq. (5.2)], then

$$\omega=\check{S}_\pi\circ\omega'\circ S_{\sigma^{-1}\pi^{-1}\sigma}\,. \tag{6.10}$$

The presence, in this formula, of the permutation σ is not very astonishing.

7. THE ϵ-TRANSPOSE OF A LINEAR MAPPING

Let V and W be two Γ-graded vector spaces. It is easy to see that there exists a unique linear mapping

$$T:\ \mathrm{Lgr}(V,W)\to \mathrm{Lgr}(W^{*\mathrm{gr}},V^{*\mathrm{gr}})\,, \tag{7.1a}$$

written in the form $g\to {}^Tg$, such that

$${}^Tg(y')=\epsilon(\gamma,\eta')\,y'\circ g \tag{7.1b}$$

for all homogeneous linear mappings $g\in\mathrm{Lgr}(V,W)$ and all homogeneous linear forms $y'\in W^{*\mathrm{gr}}$. This mapping is called *ϵ-transposition*, and for any $g\in\mathrm{Lgr}(V,W)$, the mapping ${}^Tg\in\mathrm{Lgr}(W^{*\mathrm{gr}},V^{*\mathrm{gr}})$ is called the *ϵ-transpose* of g.

Obviously, the ϵ-transposition is *homogeneous of degree zero*. If U is a third Γ-graded vector space and if $h\in\mathrm{Lgr}(U,V)$ and $g\in\mathrm{Lgr}(V,W)$ are homogeneous linear mappings, we have

$${}^T(g\circ h)=\epsilon(\gamma,\eta)\,{}^Th\circ{}^Tg\,. \tag{7.2}$$

Some care is needed in connection with the ϵ-bitranspose. If ν: $V\to(V^{*\mathrm{gr}})^{*\mathrm{gr}}$ and ν': $W\to(W^{*\mathrm{gr}})^{*\mathrm{gr}}$ are the canonical homomorphisms [see Eq. (6.3)], we obtain

$${}^{TT}g\circ\nu=\nu'\circ g \tag{7.3}$$

for all $g\in\mathrm{Lgr}(V,W)$. Now suppose that V and W are finite-dimensional and that $(V^{*\mathrm{gr}})^{*\mathrm{gr}}$ and $(W^{*\mathrm{gr}})^{*\mathrm{gr}}$ are identified with V and W, respectively, by means of the *usual* canonical mappings (this will be the case if the standard matrix calculus is applied). Then Eq. (7.3) shows that

$${}^{TT}g=\epsilon(\gamma,\gamma)g \tag{7.4}$$

for all homogeneous elements $g\in\mathrm{Lgr}(V,W)$.

The following results show that our definition of the ϵ-transpose fits quite nicely with the canonical constructions discussed so far. If

$$\omega:\ W\otimes V^{*\mathrm{gr}}\to\mathrm{Lgr}(V,W)\,, \tag{7.5}$$

$$\omega^*:\ V^{*\mathrm{gr}}\otimes(W^{*\mathrm{gr}})^{*\mathrm{gr}}\to\mathrm{Lgr}(W^{*\mathrm{gr}},V^{*\mathrm{gr}}) \tag{7.6}$$

are canonical [see Eq. (6.6)], if ν' is the canonical homomorphism of W into $(W^{*\mathrm{gr}})^{*\mathrm{gr}}$ as defined in Eq. (6.3), and if s denotes the ϵ-symmetry of $W\otimes V^{*\mathrm{gr}}$ onto $V^{*\mathrm{gr}}\otimes W$ [see Eq. (5.5)], we find that

$$T\circ\omega=\omega^*\circ(\mathrm{id}\otimes\nu')\circ s\,. \tag{7.7}$$

Thus under the canonical homomorphisms ω and ω^* the ϵ-transposition corresponds to the most natural mapping of $W\otimes V^{*\mathrm{gr}}$ into $V^{*\mathrm{gr}}\otimes(W^{*\mathrm{gr}})^{*\mathrm{gr}}$ that we could think of.

Next, let $\overline{V}$ and $\overline{W}$ be two more Γ-graded vector spaces and let g: $\overline{V}\to V$ and h: $W\to\overline{W}$ be homogeneous linear mappings of degree γ and η, respectively. We define a linear mapping

$$\psi_{h,g}:\ \mathrm{Lgr}(V,W)\to\mathrm{Lgr}(\overline{V},\overline{W}) \tag{7.8a}$$

by requiring that

$$\psi_{h,g}(a)=\epsilon(\gamma,\alpha)h\circ a\circ g \tag{7.8b}$$

for all homogeneous elements $a\in\mathrm{Lgr}(V,W)$. Of course, $\psi_{h,g}$ is homogeneous of degree $\gamma+\eta$. If

$$\omega:\ W\otimes V^{*\mathrm{gr}}\to\mathrm{Lgr}(V,W)\,, \tag{7.9}$$

$$\overline{\omega}:\ \overline{W}\otimes\overline{V}^{*\mathrm{gr}}\to\mathrm{Lgr}(\overline{V},\overline{W}) \tag{7.10}$$

are the canonical homomorphisms, it is easy to see that

$$\psi_{h,g}\circ\omega=\overline{\omega}\circ(h\overline{\otimes}\,{}^Tg)\,. \tag{7.11}$$

At last, let us assume that V and W are graded L-modules. By definition of the contragredient representation we have

$$A_{V^*}=-{}^T(A_V)\quad\text{for all } A\in L\,. \tag{7.12}$$

We may now use Eq. (7.2) to show that the ϵ-transposition is a homomorphism of graded L-modules. Finally, if $\overline{V}$ and $\overline{W}$ are also graded L-modules, then if g and h are L-invariant, so is $\psi_{h,g}$.

8. THE ϵ-TRACE

Let V be a *finite-dimensional* Γ-graded vector space. We regard V as a graded $\mathrm{gl}(V,\epsilon)$-module in the obvious way.

Let

$$\omega^{-1}:\ \mathrm{Lgr}(V,V)\rightarrow V\otimes V^{*\mathrm{gr}} \tag{8.1}$$

be the canonical isomorphism. (Recall that $V^{*\mathrm{gr}} = V^*$ and $\mathrm{Lgr}(V,V) = L(V,V)$ since V is finite-dimensional. We keep the general notation in order to emphasize the gradation of these spaces.) Moreover, let

$$s:\ V\otimes V^{*\mathrm{gr}}\rightarrow V^{*\mathrm{gr}}\otimes V \tag{8.2}$$

be the ϵ-symmetry [see Eq. (5.5)] and let

$$t:\ V^{*\mathrm{gr}}\otimes V\rightarrow K \tag{8.3}$$

denote the linear form that is associated with the canonical bilinear form on $V^{*\mathrm{gr}}\times V$ [see (4.6)]. The composed mapping

$$\mathrm{Tr}_\epsilon:\ \mathrm{Lgr}(V,V)\rightarrow V\otimes V^{*\mathrm{gr}}\rightarrow V^{*\mathrm{gr}}\otimes V\rightarrow K \tag{8.4}$$

is a linear form on $\mathrm{Lgr}(V,V)$, it is called the *ϵ-trace*. Since ω^{-1}, s, and t are homogeneous of degree zero and $\mathrm{gl}(V,\epsilon)$-invariant, Tr_ϵ is likewise. Recall that the $\mathrm{gl}(V,\epsilon)$-invariance of Tr_ϵ is equivalent to the condition that

$$\mathrm{Tr}_\epsilon(\langle g,h\rangle) = 0 \tag{8.5}$$

for all $g,h\in\mathrm{Lgr}(V,V)$.

By definition, we have

$$\mathrm{Tr}_\epsilon(\omega(x\otimes x')) = \epsilon(\xi,\xi')x'(x) \tag{8.6}$$

for all homogeneous elements $x\in V$ and $x'\in V^{*\mathrm{gr}}$. To derive an explicit formula for the ϵ-trace of a general linear mapping $g\in\mathrm{Lgr}(V,V)$, let $(a_i)_{1\leqslant i\leqslant n}$ be a *homogeneous basis* of V (i.e., a basis consisting of homogeneous elements) and let $(a_j')_{1\leqslant j\leqslant n}$ denote the corresponding dual basis of $V^{*\mathrm{gr}}$:

$$a_j'(a_i) = \delta_{ij} \quad \text{for } 1\leqslant i,j\leqslant n\,. \tag{8.7}$$

If a_i is homogeneous of degree α_i, the linear form a_j' is homogeneous of degree $-\alpha_j$. Using Eq. (8.6), it is easy to show that

$$\mathrm{Tr}_\epsilon(g) = \sum_{i=1}^{n}\epsilon(\alpha_i,\alpha_i)a_i'(g(a_i))\,. \tag{8.8}$$

Note that the numbers $a_j'(g(a_i))$ are the matrix elements of g with respect to the basis $(a_i)_{1\leqslant i\leqslant n}$. Thus Tr_ϵ generalizes the well-known supertrace to the present Γ-graded setting (see also Refs. 7 and 15).

Let V and W be any two finite-dimensional Γ-graded vector spaces. Then the ϵ-trace satisfies the following rules.

(a) If p: $V\rightarrow W$ is a bijective homogeneous linear mapping of degree π, then

$$\mathrm{Tr}_\epsilon(p\circ g\circ p^{-1}) = \epsilon(\pi,\pi)\mathrm{Tr}_\epsilon(g) \tag{8.9}$$

for all $g\in\mathrm{Lgr}(V,V)$.

(b) We have

$$\mathrm{Tr}_\epsilon(g\,\overline{\otimes}\,h) = \mathrm{Tr}_\epsilon(g)\mathrm{Tr}_\epsilon(h) \tag{8.10}$$

for all $g\in\mathrm{Lgr}(V,V)$ and $h\in\mathrm{Lgr}(W,W)$.

(c) Let s denote the ϵ-symmetry of $V\otimes V$ onto itself [see Eq. (5.5)]. Then

$$\mathrm{Tr}_\epsilon(s\circ(g\,\overline{\otimes}\,h)) = \mathrm{Tr}_\epsilon(g\circ h) \tag{8.11}$$

for all $g,h\in\mathrm{Lgr}(V,V)$.

(d) For all $g\in\mathrm{Lgr}(V,V)$,

$$\mathrm{Tr}_\epsilon({}^Tg) = \mathrm{Tr}_\epsilon(g)\,, \tag{8.12}$$

where ${}^Tg$ is the ϵ-transpose of g (see Sec. 7).

Of course, the most important property of the ϵ-trace is its $\mathrm{gl}(V,\epsilon)$-invariance. This immediately implies the following proposition.

Proposition: For any finite-dimensional graded representation ρ of the ϵ Lie algebra L and any integer $n\geqslant 1$, the so-called n-linear *ϵ-trace form*

$$\psi_n^\rho(A_1,\ldots,A_n) = \mathrm{Tr}_\epsilon(\rho(A_1)\cdots\rho(A_n)) \tag{8.13}$$

on L is homogeneous of degree zero and L-invariant. If ζ is a cyclic permutation of $\{1,\ldots,n\}$, the form ψ_n^ρ is invariant under the symmetry transformation $\check{S}_\zeta$ of $\mathrm{Lgr}_n(L,\ldots,L;K)$ onto itself (see Sec. 5).

The last statement means that, *in the graded sense*, the form ψ_n^ρ is invariant under cyclic permutations of its arguments.

In general, the proposition provides us with a multitude of invariant multilinear forms on an ϵ Lie algebra. We consider some examples.

If L is finite-dimensional, it can be applied to the adjoint representation. The case $n = 2$ then yields the so-called *Killing form* ϕ of L,

$$\phi(A,B) = \mathrm{Tr}_\epsilon((\mathrm{ad}\,A)(\mathrm{ad}\,B)) \tag{8.14}$$

for all $A,B\in L$.

To construct another example, let V be a finite-dimensional Γ-graded vector space. Then the proposition shows that the bilinear form ψ on $\mathrm{gl}(V,\epsilon)$, defined by

$$\psi(A,B) = \mathrm{Tr}_\epsilon(AB) \tag{8.15}$$

for all $A,B\in\mathrm{gl}(V,\epsilon)$, is homogeneous of degree zero, ϵ-symmetric, and $\mathrm{gl}(V,\epsilon)$-invariant; furthermore, it is easy to see that ψ is *nondegenerate*.

In fact, let ω denote the canonical isomorphism of $V\otimes V^{*\mathrm{gr}}$ onto $\mathrm{Lgr}(V,V)$. Then

$$\omega(x\otimes x')\circ\omega(y\otimes y') = x'(y)\omega(x\otimes y') \tag{8.16}$$

and hence

$$\psi(\omega(x\otimes x'),\,\omega(y\otimes y')) = \epsilon(\xi,\,\eta')x'(y)y'(x)\,, \tag{8.17}$$

for all homogeneous elements x, $y\in V$ and x', $y'\in V^{*\mathrm{gr}}$. Our claim now follows by inserting for x, y and x', y' the elements of a homogeneous basis of V and the corresponding dual basis of $V^{*\mathrm{gr}}$.

We shall next calculate the Killing form of $\mathrm{gl}(V,\epsilon)$. Recall that the canonical mapping ω is a graded $\mathrm{gl}(V,\epsilon)$-module isomorphism of $V\otimes V^{*\mathrm{gr}}$ onto $\mathrm{gl}(V,\epsilon)$. Consequently, it suffices to calculate the bilinear ϵ-trace form corresponding to $V\otimes V^{*\mathrm{gr}}$. But an element $A\in\mathrm{gl}(V,\epsilon)$ acts on $V\otimes V^{*\mathrm{gr}}$ as $A\,\overline{\otimes}\,\mathrm{id} - \mathrm{id}\,\overline{\otimes}\,{}^TA$, where ${}^TA$ denotes the ϵ-transpose of A. It is now easy to see that the Killing form ϕ_{gl} of $\mathrm{gl}(V,\epsilon)$ is given by

$$\phi_{\mathrm{gl}}(A,B) = 2d\,\mathrm{Tr}_\epsilon(AB) - 2\,\mathrm{Tr}_\epsilon(A)\,\mathrm{Tr}_\epsilon(B) \tag{8.18}$$

for all $A,B\in\mathrm{gl}(V,\epsilon)$, with

$$d = \mathrm{Tr}_\epsilon(\mathrm{id}_V)\,. \tag{8.19}$$

The integer d will play a crucial role in the following. Note that id is orthogonal to $\mathrm{gl}(V,\epsilon)$ with respect to ϕ_{gl}. This is obvious since $K\cdot\mathrm{id}$ is the center of $\mathrm{gl}(V,\epsilon)$.

Finally, let us define the *special linear ϵ Lie algebra*

$\mathrm{sl}(V,\epsilon)$ of V:

$$\mathrm{sl}(V,\epsilon) = \{A \in \mathrm{gl}(V,\epsilon) | \mathrm{Tr}_\epsilon(A) = 0\} . \tag{8.20}$$

Obviously, Eq. (8.5) implies that $\mathrm{sl}(V,\epsilon)$ is a graded ideal of $\mathrm{gl}(V,\epsilon)$. It is not difficult to prove that

$$\mathrm{sl}(V,\epsilon) = \langle \mathrm{gl}(V,\epsilon), \mathrm{gl}(V,\epsilon) \rangle \tag{8.21}$$

where, according to common usage, the right-hand side denotes the subspace of $\mathrm{gl}(V,\epsilon)$ generated by all products $\langle A,B \rangle$, with $A,B \in \mathrm{gl}(V,\epsilon)$.

We remark that id is an element of $\mathrm{sl}(V,\epsilon)$ if and only if $d = 0$. Consequently, the restriction of ψ to $\mathrm{sl}(V,\epsilon)$ is nondegenerate if and only if $d \neq 0$ (provided that $V \neq \{0\}$). Since $\mathrm{sl}(V,\epsilon)$ is a graded ideal of $\mathrm{gl}(V,\epsilon)$, its Killing form ϕ_{sl} is equal to the restriction of ϕ_{gl} to $\mathrm{sl}(V,\epsilon)$. It follows that

$$\phi_{\mathrm{sl}}(A,B) = 2d \, \mathrm{Tr}_\epsilon(AB) \tag{8.22}$$

for all $A,B \in \mathrm{sl}(V,\epsilon)$.

If d is nonzero, the adjoint $\mathrm{gl}(V,\epsilon)$-module is the direct sum of the graded submodules $\mathrm{sl}(V,\epsilon)$ and $K \cdot \mathrm{id}$. Correspondingly, the unique linear mapping

$$\omega_0\colon \ V \otimes V^{*\mathrm{gr}} \to \mathrm{sl}(V,\epsilon) \tag{8.23a}$$

such that

$$\omega_0(x \otimes x') = \omega(x \otimes x') - (1/d)\epsilon(\xi,\xi')x'(x)\mathrm{id} \tag{8.23b}$$

for all homogeneous elements $x \in V$ and $x' \in V^{*\mathrm{gr}}$, is a graded $\mathrm{gl}(V,\epsilon)$-module homomorphism of $V \otimes V^{*\mathrm{gr}}$ onto $\mathrm{sl}(V,\epsilon)$.

The case $d = 0$ but $V \neq \{0\}$ is somewhat pathological. This is apparent already from our previous remarks. Moreover, in that case there is no graded $\mathrm{sl}(V,\epsilon)$-submodule of $\mathrm{gl}(V,\epsilon)$ which is complementary to $\mathrm{sl}(V,\epsilon)$, i.e., there is no element $A \in \mathrm{gl}(V,\epsilon)_0$ such that $\langle \mathrm{sl}(V,\epsilon), A \rangle \subset K \cdot A$ and $\mathrm{Tr}_\epsilon(A) \neq 0$. Consequently, a homomorphism analogous to (8.23) does not exist.

9. THE ϵ-ADJOINT OF A LINEAR MAPPING

Throughout this section, V denotes a *finite-dimensional* Γ-graded vector space which is endowed with a nondegenerate homogeneous bilinear form b of degree β.

It is easy to see that there exists a unique linear mapping of $\mathrm{Lgr}(V,V)$ into itself, written in the form $g \to g^*$, such that

$$b(g^*(x), y) = \epsilon(\gamma,\xi) b(x, g(y)) \tag{9.1}$$

for all homogeneous elements $g \in \mathrm{Lgr}(V,V)$ and $x, y \in V$. For any $g \in \mathrm{Lgr}(V,V)$, the mapping g^* is called the *ϵ-adjoint* of g with respect to b.

The mapping $g \to g^*$ is homogeneous of degree zero and bijective; it is closely related to the ϵ-transposition. In fact, let

$$f\colon \ V \to V^{*\mathrm{gr}} \tag{9.2a}$$

be the linear mapping which is mapped onto b by the canonical isomorphism λ_1 [see Eq. (6.1)], i.e.,

$$(f(x))(y) = b(x, y) \tag{9.2b}$$

for all $x, y \in V$. We know that f is bijective and homogeneous of degree β. A brief calculation then shows that

$$g^* = \epsilon(\beta,\gamma) f^{-1} \circ {}^T g \circ f \tag{9.3}$$

for all homogeneous elements $g \in \mathrm{Lgr}(V,V)$, where ${}^T g$ is the ϵ-transpose of g.

We can now prove that the ϵ-adjoint operation satisfies

$$(g \circ h)^* = \epsilon(\gamma, \eta) h^* \circ g^* \tag{9.4}$$

for all homogeneous elements $g, h \in \mathrm{Lgr}(V,V)$, and

$$\mathrm{Tr}_\epsilon(g^*) = \epsilon(\beta,\beta) \, \mathrm{Tr}_\epsilon(g) \tag{9.5}$$

for all $g \in \mathrm{Lgr}(V,V)$; moreover, we have

$$g^{**} = g \tag{9.6}$$

for all $g \in \mathrm{Lgr}(V,V)$, *provided* that b is ϵ-symmetric or ϵ-skew-symmetric.

10. ϵ LIE ALGEBRAS LEAVING INVARIANT A BILINEAR FORM

Throughout this section, V denotes a *finite-dimensional* Γ-graded vector space which is endowed with a nondegenerate homogeneous bilinear form b of degree β. We assume that b is either *ϵ-symmetric or ϵ-skew-symmetric*; let us agree that the upper (resp. lower) sign always corresponds to the former (resp. latter) case; thus

$$b(x,y) = \pm \epsilon(\xi, \eta) b(y,x) \tag{10.1}$$

for all homogeneous elements $x, y \in V$.

A. The ϵ Lie algebras $L(b)$

Let $L(b)$ denote the graded subalgebra of $\mathrm{gl}(V,\epsilon)$ consisting of all elements which leave the bilinear form b invariant (see the end of Sec. 2).[16] Thus a homogeneous element $A \in \mathrm{gl}(V,\epsilon)$ belongs to $L(b)$ if and only if

$$b(Ax, y) + \epsilon(\alpha,\xi) b(x, Ay) = 0 \tag{10.2}$$

for all homogeneous elements $x, y \in V$. In view of the definition of the ϵ-adjoint linear mapping (with respect to b) this means that

$$L(b) = \{A \in \mathrm{gl}(V,\epsilon) | A^* = -A\} . \tag{10.3}$$

To gain some insight into the structure of $L(b)$ let us introduce the composed linear mapping

$$\pi_0\colon \ V \otimes V \to V \otimes V^{*\mathrm{gr}} \to \mathrm{Lgr}(V,V) , \tag{10.4a}$$

where the first mapping is equal to $\mathrm{id} \,\overline{\otimes}\, f$, with f defined by equation (9.2), and the second is the canonical isomorphism. It follows that

$$\pi_0(x \otimes y)z = \epsilon(\beta,\xi) b(y,z)x \tag{10.4b}$$

for all homogeneous elements $x, y, z \in V$. By definition, the mapping π_0 is bijective, homogeneous of degree β, and $L(b)$-invariant.

We are interested in the inverse image of $L(b)$ under π_0. Let s denote the ϵ-symmetry of $V \otimes V$ onto itself (see equation (5.5)). Then it is easy to see that

$$\pi_0(u)^* = \pm \epsilon(\beta,\beta) \pi_0(s(u)) \tag{10.5}$$

for all tensors $u \in V \otimes V$ (check the formula for decomposable tensors $x \otimes y$ with homogeneous elements $x, y \in V$). Consequently, for any $u \in V \otimes V$, the element $\pi_0(u)$ belongs to $L(b)$ if and only if

$$s(u) = \mp \epsilon(\beta,\beta) u . \tag{10.6}$$

We set

$$\delta = \mp \epsilon(\beta,\beta) \tag{10.7}$$

and define for $\sigma\in\{1,-1\}$

$$U^{\sigma}=\{u\in V\otimes V\,|\,s(u)=\sigma u\}\,. \tag{10.8}$$

Obviously, U^{1} and U^{-1} are graded $L(b)$-submodules of $V\otimes V$, their sum is direct and equal to $V\otimes V$, and their dimensions are given by

$$\dim U^{\sigma}=\tfrac{1}{2}(m^2+\sigma d)\,, \tag{10.9}$$

with

$$m=\dim V,\quad d=\mathrm{Tr}_{\epsilon}(\mathrm{id}_V)\,. \tag{10.10}$$

We remark that

$$d=0\quad \text{if } \epsilon(\beta,\beta)=-1\,. \tag{10.11}$$

Using this notation, our above result means that π_0 induces a bijective $L(b)$-invariant linear mapping of U^{δ} onto $L(b)$, which is homogeneous of degree β. In particular, we have

$$\dim L(b)=\tfrac{1}{2}[m^2\mp\epsilon(\beta,\beta)d\,]\,. \tag{10.12}$$

We may now compose the projector $\frac{1}{2}(\mathrm{id}+\delta s)$ of $V\otimes V$ onto U^{δ} (parallel to $U^{-\delta}$) with the mapping π_0. Thus let π denote the unique linear mapping

$$\pi\colon V\otimes V\to L(b) \tag{10.13a}$$

such that

$$\pi(x\otimes y)z=\epsilon(\beta,\xi)b(y,z)x\mp\epsilon(\beta,\beta)\epsilon(\xi,\eta)\epsilon(\beta,\eta)b(x,z)y \tag{10.13b}$$

for all homogeneous elements x, y, $z\in V$. Then π is homogeneous of degree β and $L(b)$-invariant, it maps U^{δ} bijectively onto $L(b)$, and its kernel is equal to $U^{-\delta}$. In particular, we have

$$\pi(x\otimes y)=\mp\epsilon(\beta,\beta)\epsilon(\xi,\eta)\pi(y\otimes x) \tag{10.14}$$

for all homogeneous elements x, $y\in V$. The mapping π provides us with a very useful parametrization of the algebra $L(b)$. For example, the commutation relations for $L(b)$ follow immediately from the $L(b)$-invariance of π.

Finally, let us calculate the ϵ-trace of the elements $\pi(x\otimes y)$. It is not difficult to show that for all x, $y\in V$

$$\mathrm{Tr}_{\epsilon}(\pi_0 s(x\otimes y))=b(x,y) \tag{10.15}$$

and hence that

$$\mathrm{Tr}_{\epsilon}(\pi(x\otimes y))=\pm(1-\epsilon(\beta,\beta))b(x,y)\,. \tag{10.16}$$

We shall now distinguish two cases.

(a) Suppose first that $\epsilon(\beta,\beta)=1$, i.e., that β is even. This case generalizes the orthosymplectic Lie superalgebras, and hence we shall frequently write osp(b) instead of $L(b)$. Equation (10.16) shows that

$$\mathrm{Tr}_{\epsilon}(A)=0\quad\text{for all } A\in\mathrm{osp}(b)\,, \tag{10.17}$$

a relation which also follows from Eqs. (10.3) and (9.5).

(b) Suppose next that $\epsilon(\beta,\beta)=-1$, i.e., that β is odd. Then the elements of $L(b)$ are not necessarily ϵ-traceless, provided that $V\neq\{0\}$. Let us define

$$P(b)=\{A\in L(b)\,|\,\mathrm{Tr}_{\epsilon}(A)=0\}\,. \tag{10.18}$$

Obviously, $P(b)$ is a graded ideal of $L(b)$. It can be shown that, for $V\neq\{0\}$ there is no graded $P(b)$-submodule of $L(b)$ which is complementary to $P(b)$. Our notation indicates that the algebras $P(b)$ generalize the Lie superalgebras denoted by $P(n-1)$ in Ref. 1 and by $b(n)$ in Ref. 2.

Example: We choose $\Gamma=Z_2\times Z_2$ and define

$$\epsilon((\alpha_1,\alpha_2),(\beta_1,\beta_2))=(-1)^{\alpha_1\beta_2+\alpha_2\beta_1} \tag{10.19}$$

for all $\alpha_1,\alpha_2,\beta_1,\beta_2\in Z_2$. As an abbreviation, we set $\Gamma_*=\Gamma-\{0\}$. Let V be a three-dimensional vector space. Choose a basis $(e_\alpha)_{\alpha\in\Gamma_*}$ of V and define a Γ-gradation of V by

$$V_0=\{0\}\,,\quad V_\alpha=K\cdot e_\alpha\quad\text{for } \alpha\in\Gamma_*\,. \tag{10.20}$$

Let b denote the bilinear form on V which satisfies

$$b(e_\alpha,e_\gamma)=\delta_{\alpha\gamma}\quad\text{for all } \alpha,\gamma\in\Gamma_*\,. \tag{10.21}$$

Obviously, b is nondegenerate, ϵ-symmetric, and homogeneous of degree zero.

The corresponding orthosymplectic algebra osp(b) is easily described. Define a family $(E_\eta)_{\eta\in\Gamma}$ of elements of osp(b) through the equation

$$\pi(e_\alpha\otimes e_\gamma)=E_{\alpha+\gamma}\quad\text{for all } \alpha,\gamma\in\Gamma_* \tag{10.22}$$

(this is possible). By definition, E_η is homogeneous of degree η. The element E_0 is equal to zero, whereas $(E_\alpha)_{\alpha\in\Gamma_*}$ is a basis for osp(b). Finally, we have

$$\langle E_\alpha,E_\gamma\rangle=E_{\alpha+\gamma}\quad\text{for all } \alpha,\gamma\in\Gamma_*\,. \tag{10.23}$$

Note that this algebra has already been discussed in Ref. 8.

B. The coadjoint module of $L(b)$

We define for $\sigma\in\{1,-1\}$

$$W^{\sigma}=\{A\in\mathrm{Lgr}(V,V)\,|\,A^*=\sigma A\}\,. \tag{10.24}$$

It follows that

$$W^{\sigma}=\{B+\sigma B^*\,|\,B\in\mathrm{Lgr}(V,V)\} \tag{10.25}$$

and also [see Eq. (10.5)]

$$\pi_0(U^{\sigma})=W^{\pm\sigma\epsilon(\beta,\beta)}\,. \tag{10.26}$$

In particular, we have

$$W^{-1}=L(b)\,. \tag{10.27}$$

Obviously, W^{1} and W^{-1} are Γ-graded subspaces of $\mathrm{Lgr}(V,V)$, and $\mathrm{Lgr}(V,V)$ is their direct sum. Furthermore, it is easy to check that for all $\sigma,\tau\in\{1,-1\}$

$$\langle W^{\sigma},W^{\tau}\rangle\subset W^{-\sigma\tau}\,, \tag{10.28}$$

$$\langle W^{\sigma},W^{\tau}\rangle_+\subset W^{\sigma\tau} \tag{10.29}$$

where $\langle\ ,\ \rangle_+$ denotes the ϵ-anticommutator [see Eq. (2.12)]. In particular, W^{1} is a graded $L(b)$-submodule of $\mathrm{Lgr}(V,V)$.

Now let ψ denote the bilinear form on $\mathrm{Lgr}(V,V)$ defined by

$$\psi(A,B)=\mathrm{Tr}_{\epsilon}(AB) \tag{10.30}$$

for all $A,B\in\mathrm{Lgr}(V,V)$ [see Eq. (8.15)]. We know that ψ is nondegenerate, $\mathrm{gl}(V,\epsilon)$-invariant, ϵ-symmetric, and homogeneous of degree zero. Moreover, a brief calculation (using the rules in Sec. 9) shows that

$$\psi(A,B+\sigma B^*)=\psi(A+\sigma\epsilon(\beta,\beta)A^*,B) \tag{10.31}$$

for both $\sigma\in\{1,-1\}$ and all $A,B\in\mathrm{Lgr}(V,V)$. This equation implies that $W^{-\sigma\epsilon(\beta,\beta)}$ is the subspace of $\mathrm{Lgr}(V,V)$ orthogonal to W^{σ} with respect to ψ. More precisely, for both $\sigma\in\{1,-1\}$ we draw the following conclusions:

(a) Suppose first that β is even. Then W^{σ} and $W^{-\sigma}$ are orthogonal with respect to ψ, and the restriction of ψ to W^σ is nondegenerate. In particular, the restriction of ψ to osp(b) is nondegenerate. Consequently, the coadjoint osp(b)-module (see Example 4.1) is isomorphic to the adjoint osp(b)-module.

(b) Suppose next that β is odd. Then W^σ is totally isotropic with respect to ψ (i.e., the restriction of ψ to W^σ is equal to zero), and the restriction of ψ to $W^\sigma \times W^{-\sigma}$ is nondegenerate. In particular, we may use the restriction of ψ to $W^1 \times L(b)$ to identify the graded $L(b)$-module W^1 with the coadjoint $L(b)$-module (see Example 4.1). Consequently, the dual of $P(b)$ can be identified with $W^1/K\cdot\mathrm{id}$ even when considered as a graded $L(b)$-module.

C. Some invariant multilinear forms on $L(b)$ and $L(b)^{*\mathrm{gr}}$

We keep the notation of the foregoing subsections. For any $\sigma\in\{1,-1\}$ and any integer $n\geqslant 1$ let us define an n-linear form ψ_n^σ on W^σ through the equation

$$\psi_n^\sigma(A_1,\ldots,A_n) = \mathrm{Tr}_\epsilon(A_1\ldots A_n) \tag{10.32}$$

for all $A_i\in W^\sigma$. Obviously, ψ_n^σ is homogeneous of degree zero and $L(b)$-invariant. Beside its invariance, *in the graded sense*, under cyclic permutations of its arguments (see the proposition in Sec. 8) ψ_n^σ also satisfies the relation

$$\check{S}_\rho \psi_n^\sigma = \sigma^n \epsilon(\beta,\beta)\psi_n^\sigma . \tag{10.33}$$

Here ρ is the permutation of $\{1,\ldots,n\}$ defined by $\rho(r) = n+1-r$ for $1\leqslant r\leqslant n$, and $\check{S}_\rho$ is the corresponding symmetry transformation of $\mathrm{Lgr}_n(W^\sigma,\ldots,W^\sigma;K)$ onto itself (see Sec. 5). Equation (10.33) follows from (9.4) (generalized to n factors) and (9.5).

For later reference we note that the relation (10.33) implies the vanishing of the ϵ-symmetrization of ψ_n^σ in case $\sigma^n\epsilon(\beta,\beta)$ is equal to -1.

We shall now concentrate on the invariant bilinear forms on $L(b)$. Of course, ψ_2^{-1} is nothing but the restriction of ψ to $L(b)$; we have seen that this form is nondegenerate if β is even but equal to zero if β is odd.

Let us next determine the Killing form ϕ_L of $L(b)$ [see Eq. (8.14)]. To do so we recall that π_0 induces a bijective $L(b)$-invariant linear mapping of U^δ onto $L(b)$ which is homogeneous of degree β. Consequently [see Eq. (8.9)], the Killing form of $L(b)$ is equal to $\epsilon(\beta,\beta)$ times the bilinear ϵ-trace form corresponding to U^δ. Since $V\otimes V$ is the direct sum of its graded $L(b)$-submodules U^1 and U^{-1}, and since $\frac{1}{2}(\mathrm{id}+\delta s)$ is the corresponding projector of $V\otimes V$ onto U^δ, we conclude that

$$\phi_L(A,B) = \epsilon(\beta,\beta)\mathrm{Tr}_\epsilon(\tfrac{1}{2}(\mathrm{id}+\delta s)\circ A_{V\otimes V}\circ B_{V\otimes V}) \tag{10.34}$$

for all $A,B\in L(b)$. Using our rules for the ϵ-trace (see Sec. 8) it is easy to calculate the right-hand side; we obtain

$$\phi_L(A,B) = \epsilon(\beta,\beta)((d+2\delta)\mathrm{Tr}_\epsilon(AB) + \mathrm{Tr}_\epsilon(A)\mathrm{Tr}_\epsilon(B)), \tag{10.35}$$

and hence

$$\phi_{\mathrm{osp}}(A,B) = (d\mp 2)\mathrm{Tr}_\epsilon(AB) \quad \text{if } \beta \text{ is even}, \tag{10.36}$$

$$\phi_L(A,B) = -\mathrm{Tr}_\epsilon(A)\mathrm{Tr}_\epsilon(B) \quad \text{if } \beta \text{ is odd} \tag{10.37}$$

for all $A,B\in L(b)$. In particular, the Killing form ϕ_{osp} of osp(b) (with β even) is nondegenerate if and only if $d\neq \pm 2$.

Suppose now that β is odd. Since $P(b)$ is a graded ideal of $L(b)$, its Killing form ϕ_P is equal to the restriction of ϕ_L to $P(b)$. Equation (10.37) then implies that $\phi_P = 0$.

11. CONTRACTION OF TENSORS

Let $V_1,\ldots,V_n$, $n\geqslant 2$, and W be graded L-modules. Suppose that $1\leqslant r<s\leqslant n$ and that b: $V_r\times V_s\to W$ is a homogeneous L-invariant bilinear mapping of degree β. Define a mapping τ_{rs}: $\Gamma^n\to K$ by

$$\tau_{rs}(\xi_1,\ldots,\xi_n) = \epsilon\Big(\sum_{1\leqslant i<r}\xi_i,\xi_r+\xi_s\Big)\epsilon\Big(\sum_{r<j<s}\xi_j,\xi_s\Big) \tag{11.1}$$

for all $\xi_i\in\Gamma$. Then there is a unique linear mapping

$$C_b:\ V_1\otimes\cdots\otimes V_n\to W\otimes V_1\otimes\cdots\otimes\widehat{V}_r\otimes\cdots\otimes\widehat{V}_s\otimes\cdots\otimes V_n \tag{11.2a}$$

such that

$$C_b(x_1\otimes\cdots\otimes x_n) = \tau_{rs}(\xi_1,\ldots,\xi_n)b(x_r,x_s)\otimes x_1\otimes\cdots\otimes\hat{x}_r\otimes\cdots\otimes\hat{x}_s\otimes\cdots\otimes x_n \tag{11.2b}$$

for all homogeneous elements $x_i\in V_i$; the caret indicates that the term under it has to be deleted. The mapping C_b is homogeneous of degree β and L-*invariant*, we call it a *contraction* with respect to b.

The most important case is the one with $W=K$. In that case two "independent" contractions ϵ-commute. More precisely, let r,s,r',s' be four different elements of $\{1,\ldots,n\}$ such that $r<s$ and $r'<s'$ (thus we assume that $n\geqslant 4$). If b and b' are homogeneous L-invariant bilinear forms on $V_r\times V_s$ and $V_{r'}\times V_{s'}$, of degree β and β', respectively, then

$$C_b\circ C_{b'} = \epsilon(\beta,\beta')C_{b'}\circ C_b . \tag{11.3}$$

Note that our notation is somewhat oversimplified in that on the right C_b is defined on $V_1\otimes\cdots\otimes V_n$, whereas on the left it acts on $V_1\otimes\cdots\otimes\widehat{V}_{r'}\otimes\cdots\otimes\widehat{V}_{s'}\otimes\cdots\otimes V_n$, and similarly for $C_{b'}$.

To proceed, let us introduce a second type of contraction. As before, let $V_1,\ldots,V_n$, $n\geqslant 2$, and W be graded L-modules. Suppose that $1\leqslant r<s\leqslant n$, that V_r and V_s are *finite-dimensional*, and that b is a *nondegenerate* homogeneous L-invariant bilinear form on $V_r\times V_s$ of degree β. We choose homogeneous bases $(a_p^r)_{1\leqslant p\leqslant m}$ and $(a_q^s)_{1\leqslant q\leqslant m}$ of V_r and V_s, respectively, such that

$$b(a_p^r,a_q^s) = \delta_{pq} \quad \text{for } 1\leqslant p,q\leqslant m . \tag{11.4}$$

If a_p^r and a_q^s are homogeneous of degree α_p^r and α_q^s, respectively, we have

$$\alpha_p^r + \alpha_p^s + \beta = 0 \quad \text{for } 1\leqslant p\leqslant m . \tag{11.5}$$

Then there exists a unique linear mapping

$$\check{C}_b:\ \mathrm{Lgr}_n(V_1,\ldots,V_n;W)\to\mathrm{Lgr}_{n-2}(V_1,\ldots,\widehat{V}_r,\ldots,\widehat{V}_s,\ldots,V_n;W) \tag{11.6a}$$

such that

$$(\check{C}_b(h))(x_1,\dots,\hat{x}_r,\dots,\hat{x}_s,\dots,x_n)$$
$$= \epsilon\Big(\eta + \sum_{1\leq i<r} \xi_i, \beta\Big) \sum_{p=1}^{m} \epsilon(\alpha_p^r,\alpha_p^r)\epsilon\Big(\alpha_p^s, \sum_{r<j<s} \xi_j\Big)$$
$$\times h(x_1,\dots,a_p^r,\dots,a_p^s,\dots,x_n) \tag{11.6b}$$

for all homogeneous elements $h\in\mathrm{Lgr}_n(V_1,\dots,V_n;W)$ (of degree η) and all homogeneous elements $x_i\in V_i$. Once again the caret indicates that the term under it has to be deleted.

The mapping $\check{C}_b$ is homogeneous of degree $-\beta$ and L-*invariant*, it is also called a *contraction* with respect to b.

We shall now show that this second type of contraction is closely related to the first one. Let

$$\omega:\ W\otimes V_n^{*\mathrm{gr}}\otimes\cdots\otimes V_1^{*\mathrm{gr}}\to\mathrm{Lgr}_n(V_1,\dots,V_n;W), \tag{11.7}$$

$$\omega':\ W\otimes V_n^{*\mathrm{gr}}\otimes\cdots\otimes \widehat{V}_s^{*\mathrm{gr}}\otimes\cdots\otimes \widehat{V}_r^{*\mathrm{gr}}\otimes\cdots\otimes V_1^{*\mathrm{gr}}$$
$$\to\mathrm{Lgr}_{n-2}(V_1,\dots,\widehat{V}_r,\dots,\widehat{V}_s,\dots,V_n;W) \tag{11.8}$$

be the canonical homomorphisms [see Eq. (6.5)] and let $\check{b}$ denote the ϵ-inverse of b [see Eq. (6.4)]; we recall that $\check{b}$ is a nondegenerate homogeneous L-invariant bilinear form on $V_s^{*\mathrm{gr}}\times V_r^{*\mathrm{gr}}$ of degree $-\beta$. Then we have

$$\check{C}_b\circ\omega = \omega'\circ C_{\check{b}}\,. \tag{11.9}$$

Actually, this equation has been the starting point for our definition of $\check{C}_b$. If ω and ω' are bijective (which is the case if the vector spaces V_i are all finite-dimensional), Eq. (11.9) can in fact be used to define $\check{C}_b$. In any case, it follows that $\check{C}_b$ does not depend on the choice of bases (which, of course, can also be checked directly).

We remark that two independent contractions $\check{C}_b$ and $\check{C}_{b'}$ ϵ-commute in the same sense as the contractions C_b and $C_{b'}$ above (of course, we now have to assume that V_r, V_s, $V_{r'}$, $V_{s'}$ are finite-dimensional and that b and b' are nondegenerate).

12. THE ϵ-SYMMETRIC ALGEBRA OF A GRADED L-MODULE

Let V be a graded L-module, and let $T(V)$ denote the tensor algebra of V. We recall that $T(V)$ is a $Z\times\Gamma$-graded algebra,

$$T(V) = \bigoplus_{n\in Z} T_n(V), \tag{12.1}$$

with $T_n(V)=\{0\}$ if $n\leq -1$, $T_0(V)=K$, and $T_n(V)=V\otimes\cdots\otimes V$ (n factors) if $n\geq 1$. Let $I(V,\epsilon)$ be the two-sided ideal of $T(V)$ which is generated by the tensors of the form $x\otimes y-\epsilon(\xi,\eta)y\otimes x$, where x and y are homogeneous elements of V. The quotient algebra

$$S(V,\epsilon) = T(V)/I(V,\epsilon) \tag{12.2}$$

is called the *ϵ-symmetric algebra* of V (see Ref. 6). Obviously, $I(V,\epsilon)$ is a $Z\times\Gamma$-graded ideal of $T(V)$. It follows that $S(V,\epsilon)$ is a $Z\times\Gamma$-graded algebra and that the canonical mapping

$$\tilde{\tau}:\ T(V)\to S(V,\epsilon) \tag{12.3}$$

is a homomorphism of $Z\times\Gamma$-graded algebras. We recall that $S(V,\epsilon)$ is associative, ϵ-commutative, and has a unit element.

The Z-gradation of $S(V,\epsilon)$,

$$S(V,\epsilon) = \bigoplus_{n\in Z} S_n(V,\epsilon), \tag{12.4}$$

can be made more explicit, as follows. Let us define, for all $n\in Z$,

$$I_n(V,\epsilon) = I(V,\epsilon)\cap T_n(V)\,. \tag{12.5}$$

Obviously, we have $I_n(V,\epsilon)=\{0\}$ if $n\leq 1$. For $n\geq 2$, $I_n(V,\epsilon)$ is the subspace of $T_n(V)$ that is generated by the tensors of the form

$$x_1\otimes\cdots\otimes x_r\otimes(x\otimes y-\epsilon(\xi,\eta)y\otimes x)\otimes y_1\otimes\cdots\otimes y_s\,, \tag{12.6}$$

where x, y, x_i, y_j are homogeneous elements of V and $r+s+2=n$. Thus $I_n(V,\epsilon)$ is a Γ-graded subspace of $T_n(V)$, the (direct) sum of the $I_n(V,\epsilon)$ is equal to $I(V,\epsilon)$, and $S_n(V,\epsilon)$ can be identified with $T_n(V)/I_n(V,\epsilon)$,

$$S_n(V,\epsilon) = T_n(V)/I_n(V,\epsilon)\,; \tag{12.7}$$

let

$$\tilde{\tau}_n:\ T_n(V)\to S_n(V,\epsilon) \tag{12.8}$$

be the canonical mapping. Note that $S_n(V,\epsilon)=\{0\}$ if $n\leq -1$; furthermore, $S_0(V,\epsilon)$ and $S_1(V,\epsilon)$ can be identified with K and V, respectively.

Next we recall (see Sec. 3) that $T(V)$ has a natural structure of a graded L-module. In fact, for any $A\in L$, the representative A_T is an ϵ-derivation of $T(V)$ which maps $I(V,\epsilon)$ into itself. It follows that there exists a unique graded representation $A\to A_S$ of L in $S(V,\epsilon)$ such that

$$A_S\circ\tilde{\tau} = \tilde{\tau}\circ A_T \quad \text{for all } A\in L\,. \tag{12.9}$$

For any $A\in L$, the representative A_S is the unique ϵ-derivation of the algebra $S(V,\epsilon)$ that extends the mapping A_V of $S_1(V,\epsilon)=V$ into itself. Since the $T_n(V)$, $n\in Z$, are graded L-submodules of $T(V)$, we conclude that the $S_n(V,\epsilon)$, $n\in Z$, are graded L-submodules of $S(V,\epsilon)$. By definition, $\tilde{\tau}$ and the $\tilde{\tau}_n$, $n\in Z$, are homomorphisms of graded L-modules.

The algebra $S(V,\epsilon)$ and the injection $V\to S(V,\epsilon)$ satisfy a universal property which is completely analogous to those of the usual symmetric and exterior algebras; we do not want to repeat it here (see Proposition 1 of Ref. 6). Instead, we mention a related universal pair.

For any integer $n\geq 1$ let

$$\tau_n:\ V^n\to S_n(V,\epsilon) \tag{12.10a}$$

denote the n-linear mapping associated with $\tilde{\tau}_n$, i.e.,

$$\tau_n(x_1,\dots,x_n) = x_1\cdots x_n \tag{12.10b}$$

for all $x_i\in V$. It is easy to see that τ_n is ϵ-symmetric. Then the pair $(S_n(V,\epsilon),\tau_n)$ has the following universal property:

For any ϵ-symmetric n-linear mapping f of V^n into a vector space W there exists a unique linear mapping $\hat{f}$ of $S_n(V,\epsilon)$ into W such that $f=\hat{f}\circ\tau_n$.

Now let W be a graded L-module and let $\mathrm{Lgr}_n^s(V,W;\epsilon)$ denote the graded L-submodule of all ϵ-symmetric elements of $\mathrm{Lgr}_n(V,\dots,V;W)$. Then the assignment $f\to\hat{f}$ defines a graded L-module isomorphism of $\mathrm{Lgr}_n^s(V,W;\epsilon)$ onto $\mathrm{Lgr}(S_n(V,\epsilon),W)$.

Finally, we show that $S_n(V,\epsilon)$ is isomorphic to the space of ϵ-symmetric tensors of rank n. For any integer $n\geq 1$ let $T_n^s(V,\epsilon)$ denote the graded L-submodule of all ϵ-symmetric tensors in $T_n(V)$. The ϵ-symmetrization

$$t\to\frac{1}{n!}\sum_{\pi\in\mathfrak{S}_n} S_\pi(t) \tag{12.11}$$

defines a graded L-module homomorphism of $T_n(V)$ onto $T^s_n(V,\epsilon)$. Using the universal property of $(S_n(V,\epsilon),\tau_n)$ it follows that there exists a unique surjective graded L-module homomorphism

$$\sigma_n:\ S_n(V,\epsilon)\rightarrow T^s_n(V,\epsilon) \tag{12.12a}$$

such that

$$\sigma_n(x_1\cdots x_n)=\frac{1}{n!}\sum_{\pi\in\mathfrak{S}_n} S_\pi(x_1\otimes\cdots\otimes x_n) \tag{12.12b}$$

for all $x_i\in V$. Applying $\tilde{\tau}_n$ to both sides of this equation, we see that $\tilde{\tau}_n\sigma_n(z)=z$ for all $z\in S_n(V,\epsilon)$. Thus we conclude that σ_n is a graded L-module *isomorphism* and that the restriction of $\tilde{\tau}_n$ to $T^s_n(V,\epsilon)$ is its inverse.

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Casimir elements of ϵ Lie algebras

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The classical framework for investigating the Casimir elements of a Lie algebra is generalized to the case of an ϵ Lie algebra L. We construct the standard L-module isomorphism of the ϵ-symmetric algebra of L onto its enveloping algebra, and we introduce the Harish–Chandra homomorphism. In case the generators of L can be written in a canonical two-index form, we construct the associated standard sequence of Casimir elements and derive a formula for their eigenvalues in an arbitrary highest weight module.

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1. INTRODUCTION

The present work is a direct sequel to Ref. 1. With the graded tensor calculus developed there at hand, we are now going to investigate the Casimir elements of ϵ Lie algebras[2] (and hence of Lie superalgebras[3,4]).

At present, not very much is known about this topic. Jarvis and Green[5] have constructed a standard sequence of Casimir elements for the general linear, the special linear, and the orthosymplectic Lie superalgebras and have derived certain characteristic polynomial identities. They have also calculated the eigenvalues of the quadratic Casimir operators for the irreducible finite-dimensional representations (these were already known[3]). Their investigations have been extended by Jarvis and Murray[6] to include certain algebras which are closely related to the so-called strange classical Lie superalgebras. Later on, Green and Jarvis[7] studied the ϵ Lie algebra case along similar lines. The construction of Casimir elements and the calculation of their eigenvalues have also been discussed in Refs. 8 and 9, respectively. The most profound results obtained thus far are those by Kac,[10,11] who has investigated the center of the enveloping algebra of the basic classical Lie superalgebras and, in particular, has derived a graded version of Chevalley's invariants lifting theorem (which, incidentally, only holds in a weakened form).

To study the Casimir elements of an ϵ Lie algebra, we try to follow the classical approach. It is well known[12] that the enveloping algebra $U(L)$ and the symmetric algebra $S(L)$ of a Lie algebra L are canonically isomorphic as L-modules. This implies that the center of $U(L)$ (i.e., the algebra of Casimir elements of L) is, as a vector space, isomorphic to the subspace of L-invariant elements of $S(L)$. Closely related to this is the fact that any invariant symmetric multilinear form on the coadjoint module L^* of L yields a Casimir element, provided that L is finite-dimensional. This construction may be more familiar if we assume in addition that L admits a nondegenerate invariant bilinear form, for then we may consider multilinear forms on L instead of those on L^*. As shown in the Secs. 2, 3, and 4, all these results immediately generalize to the graded case. A few elementary facts about the so-called Harish–Chandra homomorphism are derived in Sec. 5.

The aforementioned constructions are, in a sense, complete. Nevertheless, they are not quite satisfactory from a practical point of view. In the subsequent sections we shall therefore discuss a different method of constructing Casimir elements. It applies in case the generators can be written in a "canonical two-index form," but, in general, it does not yield all Casimir elements. The method is classical for Lie algebras and it has already been applied to Lie superalgebras in Refs. 5 and 6. In Sec. 6 we shall construct the corresponding algebra of "tensor operators" from which the Casimir elements are obtained via contraction. Provided that certain additional assumptions are fulfilled, we are then able to derive in Sec. 7 a general formula for the eigenvalues of these Casimir elements in a highest weight module, just as in the Lie algebra case.[13] For the generalized orthosymplectic algebras our Casimir elements satisfy certain polynomial relations, whereas for the P-type [that is, $b(n)$-type] algebras they all vanish; this will be proved in Sec. 8. A few additional remarks concerning the Casimir elements of the P-type algebras are made in Sec. 9.

Finally, in an appendix we shall briefly describe how the entries investigated in the present work behave under a change of the commutation factor.[2]

In closing this introduction we note that the conventions as specified in Ref. 1 are still in force. Thus K denotes a commutative field of characteristic zero, Γ stands for an abelian group, ϵ is a commutation factor on Γ with values in K, and L denotes an ϵ Lie algebra.

Let us also remind the reader that the degree of a homogeneous element is denoted by the "corresponding" lower case Greek letter (see the convention in Sec. 2 of Ref. 1).

2. THE CANONICAL ISOMORPHISM OF $S(L,\epsilon)$ ONTO $U(L)$

Let us first recall the definition of the (universal) enveloping algebra $U(L)$ of L.[2] We start from the tensor algebra $T(L)$ of L and consider the two-sided ideal $J(L)$ of $T(L)$ which is generated by the tensors of the form

$$A\otimes B-\epsilon(\alpha,\beta)B\otimes A-\langle A,B\rangle, \tag{2.1}$$

where A and B are homogeneous elements of L. The quotient algebra

$$U(L)=T(L)/J(L) \tag{2.2}$$

a) Supported by the Deutsche Forschungsgemeinschaft.

is called the *enveloping algebra* of L; it is associative and has a unit element. The canonical homomorphism of $T(L)$ onto $U(L)$ will be denoted by φ,

$$\varphi\colon T(L)\to U(L). \tag{2.3}$$

Next we recall that $T(L)$ is a $Z\times\Gamma$-graded algebra (see Ref. 1, Sec. 3). Since the elements (2.1) are homogeneous with respect to the Γ-gradation, it follows that $J(L)$ is a Γ-graded ideal of $T(L)$. Consequently, $U(L)$ inherits a (unique) Γ-gradation from $T(L)$ such that φ is homogeneous of degree zero. Endowed with this gradation, $U(L)$ is a Γ-graded algebra.

On the other hand, the Z-gradation of $T(L)$ leads, in general, only to a filtration of $U(L)$, as follows. For any integer n, define

$$U^n(L)=\varphi\Big(\bigoplus_{r\leqslant n}T_r(L)\Big). \tag{2.4}$$

Evidently, $(U^n(L))_{n\in Z}$ is an increasing family of Γ-graded subspaces of $U(L)$ whose union is equal to $U(L)$ and which satisfy

$$U^n(L)U^m(L)\subset U^{n+m}(L)\quad\text{for all } n,m\in Z. \tag{2.5}$$

The family $(U^n(L))_{n\in Z}$ is called the *canonical filtration* of $U(L)$. Note that $U^n(L)=\{0\}$ if $n\leqslant -1$. For any element $X\in U(L)$, the smallest integer $n\geqslant 0$ such that $X\in U^n(L)$ will be called the (filtration) *order* of X.

Evidently, the base field K can be identified with $U^0(L)$, the set of all scalar multiples of the unit element of $U(L)$. Consider next the mapping composed of the canonical injection of $L=T_1(L)$ into $T(L)$ and the canonical homomorphism φ of $T(L)$ onto $U(L)$. It follows from the Poincaré–Birkhoff–Witt theorem[2] that this mapping $L\to U(L)$ is *injective*; we use it to *identify L with a Γ-graded subspace of $U(L)$*.

To proceed we recall that the ϵ Lie algebra of ϵ-derivations of L is denoted by $D(L,\epsilon)$ (see Ref. 1, Example 2.4). We consider L as a graded $D(L,\epsilon)$-module in the obvious way. Then $T(L)$ has a natural structure of a Γ-graded $D(L,\epsilon)$-module (see Ref. 1, Sec. 3): For any $D\in D(L,\epsilon)$, the representative D_T of D is the unique ϵ-derivation of $T(L)$ which extends D. It is easy to see that the ideal $J(L)$ is invariant under all these ϵ-derivations D_T. Consequently, the representation $D\to D_T$ induces a graded representation $D\to D_U$ of $D(L,\epsilon)$ in $U(L)$ such that

$$D_U\circ\varphi=\varphi\circ D_T\quad\text{for all } D\in D(L,\epsilon). \tag{2.6}$$

Actually, D_U is the unique ϵ-derivation of $U(L)$ which extends the ϵ-derivation D of L. Since the $T_n(L)$ are graded $D(L,\epsilon)$-submodules of $T(L)$, it follows that the $U^n(L)$ are graded $D(L,\epsilon)$-submodules of $U(L)$.

For any $n\in Z$, let $T_n^s(L,\epsilon)$ denote the graded $D(L,\epsilon)$-submodule of all ϵ-symmetric tensors in $T_n(L)$ [we set $T_n^s(L,\epsilon)=T_n(L)$ if $n\leqslant 0$]. We define

$$\varphi(T_n^s(L,\epsilon))=U_n(L). \tag{2.7}$$

The homomorphism φ induces a mapping

$$\varphi_n\colon T_n^s(L,\epsilon)\to U_n(L). \tag{2.8}$$

By definition, $U_n(L)$ is a graded $D(L,\epsilon)$-submodule of $U(L)$ and φ_n is a homomorphism of graded $D(L,\epsilon)$-modules. Furthermore, the Poincaré–Birkhoff–Witt theorem[2] implies that φ_n is *bijective* and that

$$U^n(L)=\bigoplus_{r\leqslant n}U_r(L)\quad\text{for all } n\in Z. \tag{2.9}$$

Consequently, the spaces $U_n(L)$, each endowed with its Γ-gradation, yield a $Z\times\Gamma$-gradation of the *vector space* $U(L)$ (*not* of the algebra, in general). This $Z\times\Gamma$-gradation is called canonical.

It is customary to compose the mapping φ_n with the canonical $D(L,\epsilon)$-module isomorphism

$$\sigma_n\colon S_n(L,\epsilon)\to T_n^s(L,\epsilon) \tag{2.10}$$

[see Ref. 1, Sec. 12. For $n=0$ we define σ_0 through the equation $\sigma_0(1)=1$; for $n\leqslant -1$ both $S_n(L,\epsilon)$ and $T_n^s(L,\epsilon)$ are equal to $\{0\}$]. The composed mapping $\varphi_n\circ\sigma_n$ will be denoted by θ_n,

$$\theta_n\colon S_n(L,\epsilon)\to U_n(L). \tag{2.11}$$

By construction, θ_n is an isomorphism of graded $D(L,\epsilon)$-modules. For $n=0$ it is fixed by the equation $\theta_0(1)=1$; for $n\geqslant 1$ we have

$$\theta_n(A_1\cdots A_n)=\frac{1}{n!}\sum_{\pi\in\mathfrak{S}_n}\prod\epsilon(\alpha_r,\alpha_s)A_{\pi(1)}\cdots A_{\pi(n)} \tag{2.12}$$

for all homogeneous elements $A_i\in L$. Here $\mathfrak{S}_n$ is the symmetric group of $\{1,\ldots,n\}$ and the product is extended over all $r,s\in\{1,\ldots n\}$ such that $r<s$ and $\pi^{-1}(r)>\pi^{-1}(s)$. Note that the multiplication on the left of Eq. (2.12) is in $S(L,\epsilon)$ whereas on the right it is carried out in $U(L)$.

As a final step, let

$$\theta\colon S(L,\epsilon)\to U(L) \tag{2.13}$$

denote the linear mapping defined by the family $(\theta_n)_{n\in Z}$; we shall call θ the *ϵ-symmetrization*. The results obtained thus far now imply the following:

Theorem: The ϵ-symmetrization $\theta\colon S(L,\epsilon)\to U(L)$ is a canonical isomorphism of Γ-graded $D(L,\epsilon)$-modules which preserves the canonical Z-gradations.

Remark 1: The isomorphism θ has functorial properties similar to those which hold in the Lie algebra case. For example, θ is compatible with the canonical coalgebra structures of $S(L,\epsilon)$ and $U(L)$.

Remark 2: In the foregoing we have been talking about graded $D(L,\epsilon)$-modules. The reader will notice that any such module admits, in particular, a natural graded L-module structure: One simply composes the adjoint homomorphism of L into $D(L,\epsilon)$ (see Ref. 1, Example 2.4) with the graded representation of $D(L,\epsilon)$. When applied to the graded $D(L,\epsilon)$-module L, this procedure leads to the adjoint L-module. Consequently, all our statements about graded $D(L,\epsilon)$-modules imply the analogous ones for graded L-modules.

3. PARAMETRIZATION OF THE ELEMENTS OF $U(L)$ BY MULTILINEAR FORMS ON THE DUAL OF L

Throughout this section the ϵ Lie algebra L is assumed to be *finite-dimensional*.

For abbreviation, let us set for any integer $n\geqslant 1$

$$\mathrm{Fgr}_n(L^{*\mathrm{gr}})=\mathrm{Lgr}_n(L^{*\mathrm{gr}},\ldots,L^{*\mathrm{gr}};K). \tag{3.1}$$

Thus $\mathrm{Fgr}_n(L^{*\mathrm{gr}})$ is the space of all n-linear forms on the dual of L; it is endowed with a canonical structure of a graded $D(L,\epsilon)$-module.

We shall now define a linear mapping

$$C_n:\ \mathrm{Fgr}_n(L^{*\mathrm{gr}})\to U(L), \tag{3.2}$$

as follows. Consider an element $h\in\mathrm{Fgr}_n(L^{*\mathrm{gr}})$. Let $\bar h$ denote the $2n$-linear mapping of $(L^{*\mathrm{gr}})^n\times L^n$ into $U(L)$ given by

$$\bar h(A'_1,\ldots,A'_n;A_n,\ldots,A_1)=h(A'_1,\ldots,A'_n)A_n\cdots A_1 \tag{3.3}$$

for all $A'_i\in L^{*\mathrm{gr}}$ and $A_j\in L$. We contract this mapping n times with respect to the canonical bilinear form on $L^{*\mathrm{gr}}\times L$, proceeding from inside out, i.e., we contract first the variables A'_n and A_n, then A'_{n-1} and $A_{n-1},\ldots,$ and finally A'_1 and A_1 [see Ref. 1, Eq. (11.6)]. The emerging element of $U(L)$ is defined to be equal to $C_n(h)$.

Since the assignment $h\to\bar h$ and the contractions are homomorphisms of the appropriate graded $D(L,\epsilon)$-modules, the mapping C_n is likewise. It is easy to derive an explicit formula for $C_n(h)$. Let $(E_p)_{1\leqslant p\leqslant m}$ be a basis of L and let $(E'_q)_{1\leqslant q\leqslant m}$ denote the corresponding dual basis of $L^{*\mathrm{gr}}$, i.e.,

$$E'_q(E_p)=\delta_{pq}\quad\text{for } 1\leqslant p,q\leqslant m. \tag{3.4}$$

If $h\in\mathrm{Fgr}_n(L^{*\mathrm{gr}})$ is homogeneous of degree η, we obtain

$$C_n(h)=\epsilon(\eta,\eta)\sum_{p_1,\ldots,p_n}h(E'_{p_1},\ldots,E'_{p_n})\,E_{p_n}\cdots E_{p_1}. \tag{3.5}$$

Obviously, C_n maps $\mathrm{Fgr}_n(L^{*\mathrm{gr}})$ into $U^n(L)$. Moreover, if π is a permutation of $\{1,\ldots,n\}$ and if $\check S_\pi$ denotes the corresponding symmetry transformation on $\mathrm{Fgr}_n(L^{*\mathrm{gr}})$ (see Ref. 1, Sec. 5), we have

$$C_n(\check S_\pi(h))-C_n(h)\in U^{n-1}(L) \tag{3.6}$$

for all $h\in\mathrm{Fgr}_n(L^{*\mathrm{gr}})$. This result suggests to consider the case where h is ϵ-symmetric.

Let $\mathrm{Fgr}^s_n(L^{*\mathrm{gr}},\epsilon)$ denote the graded $D(L,\epsilon)$-submodule of all ϵ-symmetric elements of $\mathrm{Fgr}_n(L^{*\mathrm{gr}})$. Using the Poincaré–Birkhoff–Witt theorem,[2] it can be shown that the restriction of C_n to $\mathrm{Fgr}^s_n(L^{*\mathrm{gr}},\epsilon)$ is injective and that $U^n(L)$ is the direct sum of K and the images $C_r(\mathrm{Fgr}^s_r(L^{*\mathrm{gr}},\epsilon))$, with $1\leqslant r\leqslant n$.

On the other hand, it is easy to see that $C_n(\mathrm{Fgr}^s_n(L^{*\mathrm{gr}},\epsilon))$ is contained in $U_n(L)$. In view of Eq. (2.9) this implies that C_n induces by restriction a graded $D(L,\epsilon)$-module *isomorphism*

$$C^s_n:\ \mathrm{Fgr}^s_n(L^{*\mathrm{gr}},\epsilon)\to U_n(L). \tag{3.7}$$

Actually, the results of the present and the foregoing section are related even more closely. It is not difficult to construct canonical $D(L,\epsilon)$-module isomorphisms of $T_n(L)$ onto $\mathrm{Fgr}_n(L^{*\mathrm{gr}})$ and of $S_n(L,\epsilon)$ onto $\mathrm{Fgr}^s_n(L^{*\mathrm{gr}},\epsilon)$. A brief calculation then reveals that under these isomorphisms C_n corresponds to the canonical mapping $T_n(L)\to U(L)$ and C^s_n corresponds to θ_n, respectively.

We shall next comment on the special case where L admits a nondegenerate L-invariant bilinear form b which is homogeneous of degree β. Let

$$f:\ L\to L^{*\mathrm{gr}} \tag{3.8a}$$

denote the linear mapping defined by

$$(f(A))(B)=b(A,B) \tag{3.8b}$$

for all $A,B\in L$ (see Ref. 1, Sec. 6C). We know that f is bijective, L-invariant, and homogeneous of degree β.

For any integer $n\geqslant 1$, let $\mathrm{Fgr}_n(L)$ denote the space of all n-linear forms on L, endowed with its canonical structure of a graded L-module. To simplify the notation, we shall canonically identify $\mathrm{Fgr}_n(L)$ with the graded dual of $T_n(L)$ (see Ref. 1, Sec. 4), and similarly for $L^{*\mathrm{gr}}$.

The mapping

$$f^{-1}\bar\otimes\cdots\bar\otimes f^{-1}:\ T_n(L^{*\mathrm{gr}})\to T_n(L) \tag{3.9}$$

is bijective, L-invariant, and homogeneous of degree $-n\beta$. Consequently, its ϵ-transpose f_n is a bijective L-invariant linear mapping of $\mathrm{Lgr}_n(L)$ onto $\mathrm{Lgr}_n(L^{*\mathrm{gr}})$, which is homogeneous of degree $-n\beta$.

Now consider a homogeneous n-linear form l on L of degree λ. To calculate the element $C_n(f_n(l))$ of $U(L)$, let $(E_p)_{1\leqslant p\leqslant m}$ be a homogeneous basis of L and let $(F_q)_{1\leqslant q\leqslant m}$ be the corresponding dual basis of L, defined by

$$b(F_q,E_p)=\delta_{pq}\quad\text{for } 1\leqslant p,q\leqslant m. \tag{3.10}$$

If η_p denotes the degree of E_p, we obtain

$$C_n(f_n(l))=\epsilon(\lambda,\lambda)\sum_{p_1,\ldots,p_n}\prod_{r=1}^{n}\epsilon(\eta_{p_r},\beta)^r\,l(F_{p_1},\ldots,F_{p_n})E_{p_n}\cdots E_{p_1}. \tag{3.11}$$

The reader should keep in mind that under f_n the ϵ-symmetric elements of $\mathrm{Fgr}_n(L^{*\mathrm{gr}})$ correspond to the *ϵ-symmetric or ϵ-skew-symmetric* elements of $\mathrm{Fgr}_n(L)$ depending on whether β is even or odd.

4. THE ϵ-CENTER OF $U(L)$

Throughout this section we shall assume that the ϵ Lie algebra L is *finite-dimensional*.

Definition: Let L be an ϵ Lie algebra. An element of $U(L)$ which ϵ-commutes with all elements of $U(L)$ is called a (generalized) *Casimir element* of L, and the subspace $Z(L)$ of $U(L)$ consisting of all these elements is called the *ϵ-center* of $U(L)$.

Obviously, $Z(L)$ is a graded ϵ-commutative subalgebra of $U(L)$. Since the algebra $U(L)$ is generated by 1 and L, an element of $U(L)$ belongs to $Z(L)$ if and only if it ϵ-commutes with all elements of L.

Now recall that $U(L)$ is endowed with a graded L-module structure, as follows. The representative A_U of an element $A\in L$ is the unique ϵ-derivation of $U(L)$ which extends the ϵ-derivation ad A of L. This means that

$$A_U(X)=\langle A,X\rangle \tag{4.1}$$

for all $A\in L$ and $X\in U(L)$. Consequently, $Z(L)$ is just the subspace of all invariants of the graded L-module $U(L)$ (see Ref. 1, Definition 2.4).

We know that $U(L)$ is the direct sum of its graded L-submodules $U_n(L)$, $n\geqslant 0$ (see Sec. 2). Setting

$$Z_n(L)=Z(L)\cap U_n(L)\quad\text{for all } n\in Z, \tag{4.2}$$

we see that $Z_n(L)$ is the subspace of all invariants of the graded L-module $U_n(L)$, and that $Z(L)$ is the direct sum of its graded subspaces $Z_n(L)$, $n\geqslant 0$. The results obtained in Secs. 2 and 3 now imply the following.

Proposition 1: (a) Every L-invariant n-linear form h on

L^{*gr} gives rise to the Casimir element $C_n(h)$ of order $\leqslant n$. The order of $C_n(h)$ is equal to n if and only if the ϵ-symmetrization of h is different from zero.

(b) In order to find all Casimir elements of L it suffices to determine, for every integer $n \geqslant 1$, the space of invariants of one of the graded L-modules $S_n(L,\epsilon)$, $T_n^s(L,\epsilon)$, or $\mathrm{Fgr}_n^s(L^{*gr},\epsilon)$.

If L admits a homogeneous nondegenerate L-invariant bilinear form we may as well search for L-invariant multilinear forms on L (instead for those on L^{*gr}). This is useful to know since the proposition in Ref. 1, Sec. 8 provides us with a multitude of such forms.

Example: Suppose b is a nongenerate L-invariant bilinear form on L which is homogeneous of degree zero. Choose two bases $(E_p)_{1\leqslant p \leqslant m}$ and $(F_q)_{1\leqslant q\leqslant m}$ of L such that

$$b(F_q,E_p) = \delta_{pq} \quad \text{for } 1 \leqslant p,q \leqslant m. \tag{4.3}$$

Then the Casimir element $C_2(f_2(b))$, as specified in Eq. (3.11), is equal to

$$C_2(f_2(b)) = \sum_{p=1}^{m} E_pF_p. \tag{4.4}$$

Proposition 2: Let h be a Cartan subalgebra of the Lie algebra L_0. We assume that zero is not a weight of any of the h-modules L_γ, $\gamma \in \Gamma - \{0\}$. Consider an ϵ-symmetric L-invariant n-linear form f on L. If the restriction of f to h vanishes, then $f = 0$.

Proof: We may assume that the base field is algebraically closed, hence we can use the primary decomposition of L with respect to h.[14] By assumption, the primary component corresponding to the zero weight is equal to h. Now suppose that the restriction of f to h vanishes. Then it is not difficult to show by induction on r, $0 \leqslant r \leqslant n$, that

$$f(A_1,\ldots,A_r,H,\ldots,H) = 0 \tag{4.5}$$

for all $A_i \in L$ and all $H \in h$.

Corollary 1: On the assumptions specified in Proposition 2, every ϵ-symmetric L-invariant multilinear form on L is homogeneous of degree zero.

Corollary 2: We keep the assumptions specified in Proposition 2 and suppose in addition that L admits a nondegenerate L-invariant bilinear form which is homogeneous of degree zero. Then every Casimir element of L is homogeneous of degree zero.

Remark: Corollary 2 applies to all basic classical Lie superalgebras. A result analogous to Proposition 2, but for forms on L^{*gr}, can be proved for the (f,d) algebras [called $Q(n)$ by Kac[3]] and for some algebras related to these. It follows that all Casimir elements of these algebras, too, are homogeneous of degree zero. Thus among the classical simple Lie superalgebras only the P-type algebras [called $b(n)$ in Ref. 4] remain to be treated from this point of view.

5. THE HARISH–CHANDRA HOMOMORPHISM

To begin with, we shall fix some notation and assumptions which will be kept throughout the present section. As before, the ϵ Lie algebra L is supposed to be *finite-dimensional*. Let h be a Cartan subalgebra of the Lie algebra L_0. For any linear form $\lambda \in h^*$ we define

$$L^\lambda = \{A \in L \mid \langle H,A\rangle = \lambda(H)A \text{ for all } H \in h\}. \tag{5.1}$$

Obviously, L^λ is a graded subspace of L, and

$$\langle L^\lambda, L^\mu\rangle \subset L^{\lambda+\mu} \quad \text{for all } \lambda,\mu \in h^*. \tag{5.2}$$

We assume that $\mathrm{ad}(h)$ is *diagonalizable* in the sense that

$$L = \bigoplus_{\lambda \in h^*} L^\lambda \tag{5.3}$$

and that h is *self-normalizing* in the sense that

$$L^0 = h. \tag{5.4}$$

A *nonzero* element $\lambda \in h^*$ with $L^\lambda \neq \{0\}$ is called a *root* of L with respect to h.

The set of all roots will be denoted by Δ. We suppose that we are given two *disjoint* subsets Δ^+ and Δ^- of Δ such that

$$\Delta = \Delta^+ \cup \Delta^- \tag{5.5}$$

and such that the subspaces

$$L^\pm = \bigoplus_{\lambda \in \Delta^\pm} L^\lambda \tag{5.6}$$

are (graded) *subalgebras* of L.

The enveloping algebras $U(h)$ and $U(L^\pm)$ of h and $L^\pm$ will be canonically identified with subalgebras of $U(L)$. Note that $U(h)$ is nothing but the symmetric algebra of the vector space h and as such has a canonical Z-gradation.

After these preliminaries, we remark that there exists a unique linear mapping of $U(L^-) \otimes U(h) \otimes U(L^+)$ into $U(L)$ which maps $X \otimes Y \otimes Z$ onto XYZ, for all $X \in U(L^-)$, $Y \in U(h)$, and $Z \in U(L^+)$. Obviously, this mapping is homogeneous of degree zero, and the Poincaré–Birkhoff–Witt theorem[2] implies that it is *bijective*. It follows that $U(L)$ decomposes as

$$U(L) = U(h) \oplus U(h)U(L^+)L^+ \oplus L^-U(L^-)U(h) \oplus L^-U(L)L^+. \tag{5.7}$$

[According to common usage, if $W_1, W_2,\ldots, W_r$ are subspaces of $U(L)$, we denote by $W_1W_2\cdots W_r$ the subspace of $U(L)$ generated by the products $X_1X_2\cdots X_r$, with $X_s \in W_s$ for $1 \leqslant s \leqslant r$.] We point out that

$$U(h)U(L^+)L^+ \oplus L^-U(L)L^+ = U(L)L^+ \tag{5.8}$$

and

$$L^-U(L^-)U(h) \oplus L^-U(L)L^+ = L^-U(L). \tag{5.9}$$

Let π_0 denote the projector of $U(L)$ onto $U(h)$ corresponding to the decomposition (5.7). Obviously, $\pi_0(X)$ vanishes for all elements X of $U(L)$ which are homogeneous of nonzero degree. Moreover, it is easy to see that

$$\pi_0(U^n(L)) \subset U^n(h) \quad \text{for all } n \in Z. \tag{5.10}$$

If g is a homogeneous n-linear form on L^{*gr} the component of $\pi_0(C_n(g))$ of degree n (with respect to the Z-gradation) can be calculated as follows. We identify h^* with the subspace of L^* consisting of those elements which vanish on L^λ for all $\lambda \in \Delta$. If (H_p) is a basis of h and if (H'_q) denotes the corresponding dual basis of h^*, then the component of $\pi_0(C_n(g))$ in $U_n(h)$ is equal to

$$\epsilon(\gamma,\gamma) \sum_{q_1,\ldots,q_n} g(H'_{q_1},\ldots,H'_{q_n})\, H_{q_n}\cdots H_{q_1}. \tag{5.11}$$

Of course, this expression is equal to zero if the degree γ of g is different from zero.

We are mainly interested in the restriction π of π_0 onto $Z(L)$. It is classical that for semisimple Lie algebras π is an algebra isomorphism of $Z(L)$ onto the subalgebra of $U(h)$ consisting of the elements which are invariant under the "translated Weyl group." For Lie superalgebras, the situation is more complicated. We shall give sufficient conditions for π to be multiplicative and injective, but we shall not comment on the much more difficult problem of characterizing the image $\pi(Z(L))$. Some results concerning the latter problem have been obtained by Kac.[10,11]

In general, π_0 itself is not multiplicative. However, it is easy to see that the restrictions of π_0 to both of the algebras $U(h) \oplus U(L)L^+$ and $U(h) \oplus L^- U(L)$ are algebra homomorphisms.

Proposition 3: We keep the notation and assumptions specified above.

(a) Suppose that one of the following conditions is satisfied:

$(P_\pm)$ The vanishing of a linear combination $\Sigma_{\lambda\in\Delta^\pm} c_\lambda \lambda$ with integral coefficients $c_\lambda \geqslant 0$ implies that $c_\lambda = 0$ for all $\lambda \in \Delta^\pm$.

Then π is an algebra homomorphism.

(b) If L admits a nondegenerate L-invariant bilinear form which is homogeneous of degree zero, then π is injective.

Proof: (a) Concerning the multiplicativity, we shall obtain a somewhat stronger result. Let $U(L)^0$ be the centralizer of h in $U(L)$, i.e.,

$$U(L)^0 = \{X \in U(L) \mid \langle H,X\rangle = 0 \quad \text{for all } H \in h\}. \tag{5.12}$$

Obviously, $U(L)^0$ is a graded subalgebra of $U(L)$ which contains $Z(L)$ and $U(h)$.

Choose a basis of L which consists of homogeneous elements of the weight spaces L^λ, $\lambda \in \Delta \cup \{0\}$. Construct the associated Poincaré–Birkhoff–Witt basis of $U(L)$ relative to a total ordering which puts the basis elements corresponding to roots from Δ^- first, then the basis elements lying in $L^0 = h$, and finally the basis elements corresponding to roots from Δ^+. It is easy to identify subfamilies of this basis which are bases of $U(L)^0$, $U(h)$, $U(L)L^+$, and $L^- U(L)$, respectively. This shows that $U(L)^0$ is contained in $U(h) \oplus U(L)L^+$ or in $U(h) \oplus L^- U(L)$ depending on whether (P_-) or (P_+) is fulfilled. Consequently, the restriction of π_0 onto $U(L)^0$ is multiplicative.

(b) In view of Eq. (5.10) the mapping π will be injective if we can show that for any integer $n \geqslant 0$ and any homogeneous element $X \in Z_n(L)$, the component of $\pi_0(X)$ in $U_n(h)$ vanishes if and only if $X = 0$.

We may assume that $n \geqslant 1$. By assumption, L admits a nondegenerate L-invariant bilinear form b which is homogeneous of degree zero. Consequently, we may apply the discussion around Eq. (3.11) to write

$$X = C_n(f_n(l)), \tag{5.13}$$

where l is an ϵ-symmetric L-invariant homogeneous n-linear form on L. According to the expression (5.11), the component of $\pi_0(X)$ in $U_n(h)$ vanishes if and only if the restriction of l to h is equal to zero. But by Proposition 2, this means that $l = 0$.

Whenever the restriction of π_0 to $U(L)^0$ is multiplicative, we call this restriction the *Harish–Chandra homomorphism* of $U(L)^0$ into $U(h)$ (see Ref. 12).

Finally let us establish the well-known relationship between the mapping π and the eigenvalues of the Casimir operators in highest weight modules. Up to the end of this section, we shall *assume that the condition* (P_-) *of Proposition* 3(*a*) *is satisfied*.

Let V be a graded L-module. Suppose that there exist a homogeneous nonzero element $v \in V$ and a linear form $\Lambda \in h^*$ such that v generates V as an L-module, v is annihilated by L^+, and

$$Hv = \Lambda(H)v \quad \text{for all } H \in h. \tag{5.14}$$

Then we say that V is a graded L-module with *highest weight* Λ and *generator* v or, more simply, that V is a highest weight module. Our terminology is legitimate since the linear form Λ and the one-dimensional subspace $K\cdot v$ are uniquely determined by the foregoing conditions. In particular, $K\cdot v$ is the set of all elements of V which satisfy the condition (5.14) in place of v.

Many of the elementary properties of these modules, which hold in the case of semisimple Lie algebras,[12] can easily be extended to the present more general setting. For any linear form $\Lambda \in h^*$, there exists a graded L-module $M(\Lambda)$ with highest weight Λ, whose generators are homogeneous of degree zero and which is maximal in the sense that any graded L-module with highest weight Λ is, after a suitable shift of its gradation (see Example 2.7 of Ref. 1), isomorphic to a quotient of $M(\Lambda)$. The L-module $M(\Lambda)$ is uniquely fixed by these properties, up to isomorphism. It contains a unique maximal graded L-submodule $N(\Lambda)$ different from $M(\Lambda)$. Obviously, the quotient $M(\Lambda)/N(\Lambda)$ is an irreducible graded L-module $V(\Lambda)$ with highest weight Λ, and its generators are homogeneous of degree zero. Any irreducible graded L-module with highest weight Λ is isomorphic to $V(\Lambda)$, provided its gradation has been shifted appropriately.

As before, let V be a graded L-module with highest weight Λ. If ρ denotes the corresponding homomorphism of L into $\mathrm{gl}(V,\epsilon)$, we know[2] that there is a unique graded algebra homomorphism of $U(L)$ into $\mathrm{Lgr}(V,V)$ which extends ρ and maps 1 onto id_V. For simplicity, this homomorphism will also be denoted by ρ.

Now let X be a Casimir element of L which is homogeneous of degree zero. If v is a generator of V, our above remarks imply that $\rho(X)v$ is a scalar multiple of v. Since v generates the L-module V and since X commutes with all elements of $U(L)$, it follows that

$$\rho(X) = \chi_\rho(X)\,\mathrm{id}_V \tag{5.15}$$

with a scalar $\chi_\rho(X)$. Obviously, the assignment $X \to \chi_\rho(X)$ defines an algebra homomorphism χ_ρ of $Z(L)_0$ into K which maps 1 onto 1; it is called the *central character* of ρ.

The central character χ_ρ can be expressed in terms of the Harish–Chandra homomorphism and the highest weight Λ. To do so, we note that $U(h)$ (isomorphic to the symmetric algebra of the vector space h) can be identified with the algebra of polynomial functions on h^*. In fact, for every $\lambda\in h^*$ there exists a unique algebra homomorphism of $U(h)$ into K, which maps any element $H\in h$ onto $\lambda(H)$ and 1 onto 1. If we write this homomorphism in the form $z\to z(\lambda)$, the definition implies that

$$(H_1\cdots H_n)(\lambda) = \lambda(H_1)\cdots\lambda(H_n) \tag{5.16}$$

for all $H_i\in h$.

For any element $z\in U(h)$, we may now consider the function $\lambda\to z(\lambda)$ on h^* with values in K. This function is polynomial in the sense that it depends polynomially on the coordinates of λ with respect to any fixed basis of h^*. Moreover, it is well known (and easy to see) that the assignment just constructed defines an *isomorphism* of the algebra $U(h)$ onto the algebra of polynomial functions on h^*.

To determine χ_ρ, we recall that the condition (P_-) is satisfied, which implies that $Z(L)$ is contained in $U(h) \oplus U(L)L^+$ [see the proof of Proposition 3(a)]. This enables us to calculate the action of a Casimir element on a generator of V, with the result that

$$\chi_\rho(X) = (\pi(X))(\Lambda) \quad \text{for all } X\in Z(L)_0. \tag{5.17}$$

Note that the central character of a highest weight module depends only on the highest weight. Thus we may also write χ_Λ instead of χ_ρ.

Remark: In closing this section we would like to draw the reader's attention to some limitations of the foregoing discussion, even for the classical simple Lie superalgebras. Obviously, the (f,d) algebras [i.e., the algebras $Q(n)$] do not satisfy the requirement (5.4) that h be self-normalizing in L. Moreover, the conditions (P_+) and (P_-) rule out the $P(n)$ algebras [i.e., the $b(n)$ algebras] as well as the algebras $\mathrm{spl}(n,n)$/center, at least for the most natural choices for Δ^+ and Δ^-. Things are even worse if we pass to more general groups Γ. Even for a simple orthosymplectic algebra it may then happen that $L_0 = \{0\}$ (see the example in Sec. 10A of Ref. 1).

6. AN ALGEBRA OF BILINEAR MAPPINGS

In spite of their importance for the general theory, the results of the previous sections are of limited applicability in practical calculations. This is mainly due to the fact that for a given Casimir element it may be quite hard to determine its image under the Harish–Chandra homomorphism. We are now going to present another method to construct Casimir elements; it applies "if the generators of L can be written in a canonical two-index form." This method suffers from the drawback that, in general, it does not yield all Casimir elements, but it has the great advantage that for a Casimir element obtained this way a closed formula can be derived for its eigenvalues in highest weight modules.

To begin with let us introduce the *notation* which will be *kept throughout the subsequent sections*. As before, L denotes a *finite-dimensional* ϵ Lie algebra. We consider two finite-dimensional graded L-modules V and W, and we suppose that we are given a nondegenerate L-invariant bilinear form b on $W\times V$ which is homogeneous of degree β.

To perform contractions with respect to b (see Ref. 1, Sec. 11) we choose homogeneous bases $(e_i)_{i\in I}$ of V and $(a_j)_{j\in I}$ of W such that

$$b(a_j,e_i) = \delta_{ij} \quad \text{for all } i,j\in I. \tag{6.1}$$

Here I is a suitable finite index set. The degree of e_i is denoted by η_i, that of a_j by α_j; hence

$$\eta_i + \alpha_i + \beta = 0 \quad \text{for all } i\in I. \tag{6.2}$$

Now let S be a Γ-graded algebra. We assume that we are given a graded algebra homomorphism of L into $D(S,\epsilon)$, i.e., we assume that S is endowed with a graded L-module structure such that the elements of L act as ϵ-derivations (see Example 2.4 in Ref. 1). Examples of such algebras are the enveloping algebra $U(L)$ and the algebras $\mathrm{Lgr}(U,U)$ with U a graded L-module.

We introduce in $\mathrm{Lgr}_2(V,W;S)$ a (bilinear) multiplication, denoted by an asterisk. Of course, it is sufficient to define $t*t'$ for homogeneous elements t and t' of $\mathrm{Lgr}_2(V, W; S)$. As an intermediate step, consider the quadrilinear mapping $t\times t'$ of $V\times W\times V\times W$ into S given by

$$(t\times t')(x,y,x',y') = \epsilon(\tau',\xi+\eta)t(x,y)t'(x',y') \tag{6.3}$$

for all homogeneous elements $x,x'\in V$ and $y,y'\in W$. Contraction of the second and third variable with respect to b then yields the product mapping

$$t*t'\colon\ V\times W\to S; \tag{6.4a}$$

it satisfies

$$(t*t')(x,y) = \epsilon(\tau+\tau'+\xi,\beta)\epsilon(\tau',\xi)$$
$$\times\sum_{i\in I}\epsilon(\tau'+\alpha_i,\alpha_i)t(x,a_i)t'(e_i,y) \tag{6.4b}$$

for all homogeneous elements $x\in V$ and $y\in W$. Note that $t*t'$ is homogeneous of degree $\tau+\tau'-\beta$. Thus the $*$ multiplication is homogeneous of degree $-\beta$ and does not, in general, convert $\mathrm{Lgr}_2(V,W;S)$ into a Γ-graded algebra. Actually, this could be redressed by shifting the gradation of $\mathrm{Lgr}_2(V,W;S)$, but we shall not do this.

Let us next derive some of the properties of the $*$ multiplication. The assignment $(t,t')\to t\times t'$ [bilinearly extended to all elements t and t' of $\mathrm{Lgr}_2(V,W;S)$] is homogeneous of degree zero and the contraction is homogeneous of degree $-\beta$; moreover, both of these mappings are L-invariant. Consequently, the $*$ multiplication is homogeneous of degree $-\beta$ and L-invariant. In particular, *if t and t' are two L-invariant elements of* $\mathrm{Lgr}_2(V,W;S)$, *so is $t*t'$.*

If the algebra S is associative, then the $*$ multiplication is "associative up to a factor" in the sense that

$$(t*t')*t'' = \epsilon(\tau-\beta,\beta)t*(t'*t'') \tag{6.5}$$

for all homogeneous elements $t, t', t''\in\mathrm{Lgr}_2(V,W;S)$.

Let us next introduce the bilinear form sb on $V\times W$, defined by

$$sb(x,y) = \epsilon(\xi,\eta)b(y,x) \tag{6.6}$$

for all homogeneous elements $x\in V$ and $y\in W$ (see Example 5.2 in Ref. 1). Like b itself, sb is nondegenerate, L-invariant, and homogeneous of degree β.

If S has a unit element, we may consider sb a bilinear mapping of $V\times W$ into S. Then the $*$ multiplication with sb is well-defined, and we obtain

$$(sb)*t = t, \quad t*(sb) = \epsilon(\tau-\beta,\beta)t \tag{6.7}$$

for all homogeneous elements $t \in \mathrm{Lgr}_2(V,W;S)$.

Remark: Obviously, the homogeneous component $\mathrm{Lgr}_2(V,W;S)_\beta$ is a subalgebra of $\mathrm{Lgr}_2(V,W;S)$. The above results show that if S is associative and has a unit element, then the same holds for $\mathrm{Lgr}_2(V,W;S)_\beta$. Note also that for elements $t,t' \in \mathrm{Lgr}_2(V,W;S)_\beta$ the ϵ factors in front of the sum in Eq. (6.4b) cancel.

Finally, every element of $\mathrm{Lgr}_2(V,W;S)$ can be contracted with respect to sb. This yields the linear mapping

$$[\quad]: \mathrm{Lgr}_2(V,W;S) \rightarrow S, \tag{6.8a}$$

with

$$[t] = \epsilon(\tau-\beta,\beta)\sum_{i\in I}\epsilon(\beta,\alpha_i)t(e_i,a_i) \tag{6.8b}$$

for all homogeneous elements $t \in \mathrm{Lgr}_2(V,W;S)$. We know that this mapping is homogeneous of degree $-\beta$ and L-invariant. In particular, $[sb] = \mathrm{Tr}_\epsilon(\mathrm{id}_W)$ if S has a unit element.

7. EIGENVALUES OF CASIMIR OPERATORS

When applied to the algebra $S = U(L)$, the results of the foregoing section provide us with a simple method for constructing Casimir elements: Choose a homogeneous L-invariant bilinear mapping t of $V \times W$ into $U(L)$, calculate the n^{th} $*$power of t, for example, in the form $(\cdots((t*t)*t)*\cdots)*t$, n factors t, and contract with respect to sb. For any integer $n \geqslant 1$, this leads to the following Casimir element of L

$$\begin{aligned} C_n^t &= \epsilon(\tau-\beta,\beta)^{n(n+1)/2} \\ &\quad\times \sum_{i_1,\ldots,i_n}\epsilon(\tau+\alpha_{i_1},\alpha_{i_1})\cdots\epsilon(\tau+\alpha_{i_{n-1}},\alpha_{i_{n-1}}) \\ &\quad\times\epsilon(n\beta-(n-1)\tau,\alpha_{i_n})t(e_{i_n},a_{i_1})t(e_{i_1},a_{i_2})\cdots t(e_{i_{n-1}},a_{i_n}); \end{aligned} \tag{7.1}$$

it is homogeneous of degree $n(\tau-\beta)$.

In the following, we shall restrict our attention to the case where

$$t: V \times W \rightarrow L \tag{7.2}$$

is an L-invariant bilinear mapping of $V \times W$ into L, which is homogeneous of degree β.

Example 1: Choose $W = V^{*\mathrm{gr}}$ and let b be the canonical bilinear form on $V^{*\mathrm{gr}} \times V$. Then Eqs. (6.6) and (8.23) of Ref. 1 provide mappings of $V \times V^{*\mathrm{gr}}$ into $\mathrm{gl}(V,\epsilon)$ and $\mathrm{sl}(V,\epsilon)$, respectively, which meet our requirements. [In the latter case, we have to assume that $\mathrm{Tr}_\epsilon(\mathrm{id}_V) \neq 0$.]

Example 2: Choose $W = V$ and $L = L(b)$ (see Ref. 1, Sec. 10). Then Eq. (10.13) of Ref. 1 yields a mapping $V \times V \rightarrow L(b)$, which satisfies our conditions.

Example 3: The following example is taken from Ref. 6. Suppose f is a graded algebra automorphism of $\mathrm{gl}(V,\epsilon)$ with $f^2 = \mathrm{id}$. Let $L \subset \mathrm{gl}(V,\epsilon)$ be the algebra of fixed points of f. Then the canonical mapping of $V \times V^{*\mathrm{gr}}$ into $\mathrm{gl}(V,\epsilon)$, composed with $(f + \mathrm{id})$, is a mapping $V \times V^{*\mathrm{gr}} \rightarrow L$ of the type in question. (Of course, b is chosen to be the canonical bilinear form on $V^{*\mathrm{gr}} \times V$.) Note that Example 2 is essentially a special case of the present one: Simply choose $f(A) = -A^*$ for all $A \in \mathrm{gl}(V,\epsilon)$, where A^* is the ϵ-adjoint of A with respect to b (see Ref. 1, Sec. 9).

Let us next introduce some assumptions and notation which enable us to calculate the eigenvalue of C_n^t in a "highest weight module."

(a) Choose a Cartan subalgebra h of the Lie algebra L_0. We assume that the h-modules V and W are the (necessarily direct) sums of their weight subspaces and that the weights of these modules all have a multiplicity equal to one.

(b) Now recall that the bilinear form b is nondegenerate and h-invariant. According to (a), we conclude that there exists a family $(\lambda_i)_{i\in I}$ of *different* linear forms on h such that $\{\lambda_i | i \in I\}$ and $\{-\lambda_i | i\in I\}$ are the sets of weights of the h-modules V and W, respectively. Since h is contained in L_0, we may, therefore, assume without loss of generality that the bases $(e_i)_{i\in I}$ and $(a_j)_{j\in I}$ are chosen such that e_i and a_j are weight vectors corresponding to the weights λ_i and $-\lambda_j$, respectively.

It follows that for all $i,j \in I$ the element $t(e_i,a_j)$ is homogeneous of degree $\eta_i - \eta_j$ and satisfies

$$\langle H, t(e_i,a_j)\rangle = (\lambda_i - \lambda_j)(H)t(e_i,a_j) \tag{7.3}$$

for all $H \in h$. In particular, we have

$$t(e_i,a_i) \in h \quad \text{for all } i \in I. \tag{7.4}$$

(c) We choose a subset Π of $I \times I$ such that for any pair $(i,j) \in I \times I$, exactly one of the relations $(i,j) \in \Pi$, $i = j$, $(j,i) \in \Pi$ is satisfied. In our applications, there will exist a total ordering of I such that

$$\Pi = \{(i,j) | i,j \in I;\ i < j\}. \tag{7.5}$$

(d) Now let M be an L-module. The corresponding representation of L, canonically extended to $U(L)$, will be denoted by ρ. We consider a nonzero element $y \in M$ and a linear form $\Lambda \in h^*$ such that

$$\rho(H)y = \Lambda(H)y \quad \text{for all } H \in h \tag{7.6}$$

and such that $\Lambda + (\lambda_i - \lambda_j)$ is *not* a weight of the h-module M whenever $(i,j) \in \Pi$.

Under these assumptions, y is an eigenvector of the Casimir operator $\rho(C_n^t)$, and the corresponding eigenvalue can be calculated as follows (compare with Ref. 13). Consider an L-invariant bilinear mapping $t': V \times W \rightarrow U(L)$, which is homogeneous of degree β. (We are interested in the case where t' is a $*$ power of t.) Set

$$\Lambda(t(e_i,a_i)) = n_i \quad \text{for all } i \in I, \tag{7.7}$$

and define $I \times I$ matrix (ξ_{ij}) by

$$\xi_{ij} = \begin{cases} 1 & \text{if } (i,j) \in \Pi \\ 0 & \text{otherwise,} \end{cases} \tag{7.8}$$

the $I \times I$ matrix (c_{ij}) by

$$t(e_j,a_i)e_i = c_{ij}e_j \tag{7.9}$$

[this is possible since $t(e_j,a_i)e_i$ belongs to the weight λ_j] and the $I \times I$ matrix (A_{ij}) by

$$A_{ij} = \Big(\epsilon(\alpha_i,\eta_i)n_i + \sum_{k\in I}\epsilon(\alpha_k,\eta_k)\xi_{ik}c_{ik}\Big)\delta_{ij} - \epsilon(\alpha_j,\eta_j)^2\epsilon(\eta_i,\alpha_i)\xi_{ij}c_{ij}. \tag{7.10}$$

Then a straightforward calculation shows that for all $i\in I$

$$\rho((t'*t)(e_i,a_i))y = \sum_{j\in I} A_{ij}\rho(t'(e_j,a_j))y. \tag{7.11}$$

Iterating this result we obtain for the n^{th} $*$ power t^{*n} of t

$$\rho(t^{*n}(e_i,a_i))y = \sum_{j\in I}\epsilon(\eta_j,\alpha_j)(A^n)_{ij}y. \tag{7.12}$$

If we define $t^{*0} = sb$ [see Eq. (6.7)], this relation is valid even for $n = 0$.

By definition, the Casimir element $C^{\,t}_n$ is obtained from t^{*n} by contraction with respect to sb. It follows that

$$\rho(C^{\,t}_n)y = C^{\,t}_n(\Lambda)y \tag{7.13}$$

with

$$C^{\,t}_n(\Lambda) = \sum_{i,j\in I}\epsilon(\beta,\alpha_i)\epsilon(\eta_j,\alpha_j)(A^n)_{ij}. \tag{7.14}$$

Note that $C^{\,t}_0(\Lambda) = \mathrm{Tr}_\epsilon(\mathrm{id}_W)$. This agrees with our previous remark that $[sb] = \mathrm{Tr}_\epsilon(\mathrm{id}_W)$. For $n\geqslant 1$, the right-hand side of Eq. (7.14) can be slightly simplified by using

$$\sum_{j\in I}\epsilon(\eta_j,\alpha_j)A_{ij} = n_i. \tag{7.15}$$

This relation follows from Eq. (7.12) with $n = 1$, but it can also be checked directly.

The formula (7.14) has a wide range of applicability (however, see the remark at the end of Sec. 5). Nevertheless, it suffers from certain drawbacks. First of all, it is not easy to handle for higher values of n. But the main disadvantage seems to be that the symmetry properties of $C^{\,t}_n(\Lambda)$ as a function of Λ (like the invariance under the translated Weyl group in the case of semisimple Lie algebras) are not manifestly exhibited.

Equation (7.14) enables us to derive a remarkable relation for the functions $C^{\,t}_n(\Lambda)$, as follows. Let T be an indeterminate. We consider the characteristic polynomial

$$\det(T - A) = \sum_{s=0}^{r} a_s T^s \tag{7.16}$$

of the matrix $A = (A_{ij})$, with $a_r = 1$. Of course, the a_s are polynomial functions of Λ. As is well known, A satisfies its own characteristic equation, i.e.,

$$\sum_{s=0}^{r} a_s A^s = 0. \tag{7.17}$$

Consequently, Eq. (7.14) implies that for all integers $p\geqslant 0$

$$\sum_{s=0}^{r} a_s(\Lambda)C^{\,t}_{s+p}(\Lambda) = 0. \tag{7.18}$$

Thus the functions $C^{\,t}_n(\Lambda)$ with $n\geqslant r+1$ can be written as polynomials in the functions $C^{\,t}_s(\Lambda)$ and $a_s(\Lambda)$, with $0\leqslant s\leqslant r$. Regrettably, it is quite exceptional that these relations can be used to express the Casimir elements $C^{\,t}_n$ with $n\geqslant r+1$ in terms of lower-order Casimir elements (which is possible for the classical Lie algebras). The point is that, even for the basic classical Lie superalgebras, the functions $a_s(\Lambda)$ are not, in general, the eigenvalues of suitable Casimir elements in a graded representation with highest weight Λ (see Refs. 15 and 16 for further details). Nevertheless, the relations (7.18) are useful in the determination of the functions $C^{\,t}_n(\Lambda)$, especially if the dimension r of V and W is small.

8. THE SPECIAL CASE $L = L(b)$

In the present section we would like to comment on the special case $W = V$ and $L = L(b)$ (see Ref. 1, Sec. 10). We assume that b is ϵ-symmetric or ϵ-skew-symmetric. Let us agree that, in the subsequent discussion, the upper (resp. lower) sign always corresponds to the former (resp. latter) case. For any bilinear mapping f of $V\times V$ into some vector space, the bilinear mapping sf of $V\times V$ into that vector space is defined by

$$sf(x,y) = \epsilon(\xi,\eta)f(y,x) \tag{8.1}$$

for all homogeneous elements $x,y\in V$ (see Ref. 1, Example 5.2). In particular, we have

$$sb = \pm b. \tag{8.2}$$

According to Ref. 1, Sec. 10, the bilinear mapping

$$t\colon\ V\times V\to L(b), \tag{8.3a}$$

which satisfies

$$t(x,y)z = \epsilon(\beta,\xi)b(y,z)x \mp \epsilon(\beta,\beta)\epsilon(\xi,\eta)\epsilon(\beta,\eta)b(x,z)y \tag{8.3b}$$

for all homogeneous elements $x,y,z\in V$, meets all our requirements. Moreover, we know that

$$st = \mp\epsilon(\beta,\beta)t. \tag{8.4}$$

We are going to derive certain relations between the Casimir elements $C^{\,t}_n$ (see also Refs. 5 and 6).

To do so, let us first investigate the symmetry properties of the $*$ powers t^{*n} of t; recall that these powers are unambiguously defined and that $t^{*0} = sb$. Consider an $L(b)$-invariant bilinear mapping t': $V\times V\to U(L(b))$, which is homogeneous of degree β. A straightforward calculation shows that

$$s(t'*t) = \epsilon(\beta,\beta)(-t*st' + (d\mp 1)st' + t' - [t']b), \tag{8.5}$$

where

$$d = \mathrm{Tr}_\epsilon(\mathrm{id}_V) \tag{8.6}$$

and where [ ] denotes contraction with respect to sb [see Eq. (6.8)].

It is easy to check that

$$[st'] = \pm\epsilon(\beta,\beta)[t']; \tag{8.7}$$

furthermore, we have $[b] = \pm d$. Induction on n now shows that $s(t^{*n})\mp(-\epsilon(\beta,\beta))^n t^{*n}$ is a linear combination of products of the form $C^{\,t}_{p_1}\cdots C^{\,t}_{p_r}t^{*p}$, where $p,p_1,\ldots,p_r$ are integers which satisfy

$$p\geqslant 0,\quad p_i\geqslant 1,\quad 1\leqslant p + \sum_{i=1}^{r} p_i\leqslant n-1. \tag{8.8}$$

Contraction with respect to sb then implies that $(1 + (-\epsilon(\beta,\beta))^{n-1})C^{\,t}_n$ is a linear combination of products of the form $C^{\,t}_{p_1}\cdots C^{\,t}_{p_r}C^{\,t}_p$, where the integers $p,p_1,\ldots,p_r$ satisfy the conditions (8.8). In particular, it follows that

$$C_1^{\prime}=0, \tag{8.9}$$

which is obvious anyhow. The following discussion depends on whether β is even or odd.

(a) Let us first assume that β is even, $\epsilon(\beta,\beta)=1$. Then we conclude that for any integer $q\geqslant 0$ the Casimir element $C_{2q+1}^{\prime}$ is a linear combination of products of the form $C_{2q_1}^{\prime}\cdots C_{2q_r}^{\prime}$, where the q_i are integers which satisfy $q_i\geqslant 1$ and $\Sigma_{i=1}^{r} q_i\leqslant q$. In particular, we have

$$C_3^{\prime}=\tfrac{1}{2}(d\mp 2)C_2^{\prime}, \tag{8.10}$$

$$C_5^{\prime}=\tfrac{1}{2}(3d\mp 4)C_4^{\prime}\mp\tfrac{1}{2}(C_2^{\prime})^2-\tfrac{1}{4}(d\mp 1)(d\mp 2)^2C_2^{\prime}. \tag{8.11}$$

(b) Consider now the case where β is odd, $\epsilon(\beta,\beta)=-1$. Then our above result implies that the Casimir elements $C_n^{\prime}$ are all equal to zero. Using this fact (and recalling that $d=0$ in the present case), we conclude from Eq. (8.5) that

$$s(t^{*n})=\pm t^{*n}\quad\text{for all } n\geqslant 0. \tag{8.12}$$

Conversely, this equation implies that $C_n^{\prime}=0$.

9. CONCLUDING REMARKS

In the present paper we have established a framework for investigating the Casimir elements of ϵ Lie algebras. Our methods apply, in particular, to the general linear, the special linear, and the orthosymplectic Lie superalgebras; this will be shown in the subsequent paper.[15] Let us, therefore, comment on the algebras $L(b)$ and $P(b)$, with β odd (see Ref. 1, Sec. 10). The reader will notice that we have not been able to construct any nontrivial Casimir elements for these algebras. This is obvious for the preceding section: All that we have got in this case were the mappings t^{*n} whose use is completely obscure. Consequently, we try the alternative (and more fundamental) method as described in Sec. 4. Actually, we have constructed an $L(b)$-invariant n-linear form ψ_n^1 on the coadjoint module of $L(b)$, for any integer $n\geqslant 3$ (see Ref. 1, Sec. 10C). But we have stressed already that the ϵ-symmetrization of this form vanishes. Consequently, the order of the Casimir element $C_n(\psi_n^1)$ is at most equal to $n-1$. Thus even if $C_n(\psi_n^1)$ should be different from zero, its representation in terms of ψ_n^1 would be rather "uneconomical."

Let us now restrict our attention to the Lie superalgebra case, with $\frac{1}{2}\dim V\geqslant 3$ [in which case $P(b)$ is simple]. Then a straightforward analysis shows that neither $L(b)$ nor $P(b)$ has any nontrivial Casimir elements of order $\leqslant 4$. Do these algebras have any nontrivial Casimir elements at all?

Note added in proof: In a recent work, published in C. R. Acad. Bulg. Sci. **35**, 573 (1982), A. N. Sergeev has described, for various Lie superalgebras, including the general linear, the special linear, and the orthosymplectic ones, the invariants in the supersymmetric algebra of the coadjoint module.

APPENDIX: CHANGE OF THE COMMUTATION FACTOR

As has been shown in Ref. 2, for any fixed abelian group Γ of degrees, there is a simple construction which allows for a transition between ϵ Lie algebras corresponding to different commutation factors. In this appendix we are going to describe how the entries investigated in the present work behave under such a change of the commutation factor.

Let σ be a normalized multiplier on Γ, i.e., a mapping of $\Gamma\times\Gamma$ into $K-\{0\}$ such that

$$\sigma(\alpha,\beta)\sigma(\alpha+\beta,\gamma)=\sigma(\alpha,\beta+\gamma)\sigma(\beta,\gamma) \tag{A1}$$

for all $\alpha,\beta,\gamma\in\Gamma$ and

$$\sigma(0,0)=1. \tag{A2}$$

This implies that

$$\sigma(\alpha,0)=\sigma(0,\alpha)=1 \tag{A3}$$

for all $\alpha\in\Gamma$. We recall that the function δ on $\Gamma\times\Gamma$, defined by

$$\delta(\alpha,\beta)=\sigma(\alpha,\beta)\sigma(\beta,\alpha)^{-1} \tag{A4}$$

for all $\alpha,\beta\in\Gamma$, is a commutation factor on Γ.

Consider an arbitrary Γ-graded algebra S. Generalizing a construction introduced in Ref. 2, we define a new Γ-graded algebra S^{σ} by requiring that the underlying Γ-graded vector space of S^{σ} should be equal to that of S, but that the multiplication in S^{σ}, denoted by a dot, should satisfy

$$X\cdot Y=\sigma(\xi,\eta)XY \tag{A5}$$

for all homogeneous elements $X,Y\in S$ (where the right-hand side is calculated according to the original multiplication in S).

The following properties are easily established.

(a) If f is a graded algebra homomorphism of S into a second Γ-graded algebra T, then f is a graded algebra homomorphism of S^{σ} into T^{σ} as well. In particular, if S is a graded subalgebra of T, then S^{σ} can be identified with a graded subalgebra of T^{σ}.

(b) If S is associative, then so is S^{σ}.

(c) If S has a unit element E, then E is a unit element of S^{σ}.

(d) If S is an ϵ Lie algebra, then S^{σ} is an $\epsilon\delta$ Lie algebra.

(e) If S is associative and if $S(\epsilon)$ denotes the ϵ Lie algebra associated with S (see Ref. 1, Example 2.2), then the $\epsilon\delta$ Lie algebras $S(\epsilon)^{\sigma}$ and $S^{\sigma}(\epsilon\delta)$ coincide. Thus if Z denotes the ϵ-center of S, then the $\epsilon\delta$-center of S^{σ} is equal to Z^{σ}.

(f) Let V be a Γ-graded vector space. Then there exists a unique linear mapping ω of $\mathrm{Lgr}(V,V)$ into itself such that

$$\omega(A)x=\sigma(\alpha,\xi)Ax \tag{A6}$$

for all homogeneous elements $A\in\mathrm{Lgr}(V,V)$ and $x\in V$, and ω is a graded algebra isomorphism of $\mathrm{Lgr}(V,V)^{\sigma}$ onto $\mathrm{Lgr}(V,V)$. Because of (e), this implies that ω is a graded algebra isomorphism of $\mathrm{gl}(V,\epsilon)^{\sigma}$ onto $\mathrm{gl}(V,\epsilon\delta)$, too.

(g) We keep the notation of (f) but assume in addition that V is finite-dimensional. Then ω maps $\mathrm{sl}(V,\epsilon)^{\sigma}$ onto $\mathrm{sl}(V,\epsilon\delta)$. Now consider a homogeneous bilinear form b on V. Let $L(b,\epsilon)$ denote the ϵ Lie algebra consisting of all elements of $\mathrm{gl}(V,\epsilon)$ which leave b invariant (see Ref. 1, Secs. 2 and 10). Then ω maps $L(b,\epsilon)^{\sigma}$ onto $L(b^{\sigma},\epsilon\delta)$, where the homogeneous bilinear form b^{σ} on V is given by

$$b^{\sigma}(x,y)=\sigma(\xi,\eta)b(x,y) \tag{A7}$$

for all homogeneous elements $x,y\in V$. Note that if b is nondegenerate, then b^{σ} is likewise. Furthermore, if b is ϵ-symmetric or ϵ-skew-symmetric, then b^{σ} is $\epsilon\delta$-symmetric or $\epsilon\delta$-skew-symmetric, respectively.

Now let L be an ϵ Lie algebra, and let $U(L)$ be its enveloping algebra. Because of (a) and (e), the algebra $U(L)^{\sigma}$ and the canonical injection of L^{σ} into $U(L)^{\sigma}$ have the universal property which characterizes the algebra $U(L^{\sigma})$ and the canonical injection of L^{σ} into it. Consequently, the Γ-graded algebras $U(L^{\sigma})$ and $U(L)^{\sigma}$ can (and will) be identified, and then the canonical injections of L into $U(L)$ and of L^{σ} into $U(L^{\sigma})$ are just the same. According to (e), this implies that L and L^{σ} have the same Casimir elements or, more precisely, that $Z(L)^{\sigma}$ [considered as a subalgebra of $U(L)^{\sigma}$] and $Z(L^{\sigma})$ coincide as Γ-graded algebras.

Consider next a graded representation ρ of L in a Γ-graded vector space V. According to Ref. 2, this yields a graded representation ρ^{σ} of L^{σ} in V which, by definition, is equal to $\omega\circ\rho$. In view of (a) and (f), it follows that this equality holds even if ρ and ρ^{σ} are canonically extended to $U(L)$ and $U(L^{\sigma}) = U(L)^{\sigma}$, respectively. In particular, $\rho(X)$ and $\rho^{\sigma}(X)$ coincide for all elements X of $U(L)$ which are homogeneous of degree zero.

Finally, we remark that for Sec. 5 the transition from L to L^{σ} is trivial. In fact, the algebras L_0 and L_0^{σ} coincide, and for any Cartan subalgebra h of $L_0 = L_0^{\sigma}$, the adjoint actions of h on L and L^{σ} are the same [see Eq. (A3)]. Consequently, the corresponding root systems and root space decompositions of L and L^{σ} agree as well. If we choose the same sets $\Delta^{\pm}$ in both cases, then the projectors π_0 coincide, too. Moreover, if ρ is a graded highest weight representation of L, then ρ^{σ} is a graded highest weight representation of L^{σ} with the same highest weight, and the generators are also the same.

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Eigenvalues of Casimir operators for the general linear, the special linear, and the orthosymplectic Lie superalgebras

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The generators of the algebras under consideration can be written in a canonical two-index form and hence the associated standard sequence of Casimir elements can be constructed. Following the classical approach by Perelomov and Popov, we obtain the eigenvalues of these Casimir elements in an arbitrary highest weight module by calculating the corresponding generating functions.

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1. INTRODUCTION

In the two preceding papers[1,2] we have developed a graded tensor calculus and have laid the foundation for an investigation of the Casimir elements of ϵ Lie algebras.[3] We are now going to apply our results to the general linear, the special linear, and the orthosymplectic Lie superalgebras.[4,5]

Recall that the generators of these algebras can be written in a "canonical two-index form." This immediately leads to the definition of a sequence of Casimir elements for these algebras (see also Refs. 6 and 7). In Ref. 2 we have derived a general formula for the eigenvalues of these Casimir elements in a highest weight representation. It turns out that for the algebras in question this formula can be simplified considerably, just as in the classical Lie algebra case.[8] This will be the main objective of the present paper.

We intend to keep this work as self-contained as possible. The reader who is interested in physical applications should be able to use our results without having to go through the details of their derivation. Thus, for any of the algebras under consideration, we specify:

(a) the generators (written in the two-index form) from which the Casimir elements are constructed;

(b) the root system[9];

(c) a general formula for the eigenvalues of the Casimir elements in a highest weight representation and a generating function for these eigenvalues;

(d) explicit formulae for the eigenvalues of the lower-order Casimir elements.

All this will be carried out in the Secs. 2–4 (one section for each class of algebras). In Sec. 5 we consider the example of the algebra spl(2,1). This serves to point out some peculiarities of the algebra of Casimir elements.

Let us close this introduction by a few conventions which will be kept throughout the present paper. The field of scalars K is any commutative field of characteristic zero. We restrict our attention to the Z_2-graded case (with $Z_2 = Z/2Z = \{\bar{0},\bar{1}\}$ and set

$$\epsilon(\alpha,\beta) = (-1)^{\alpha\beta} \quad \text{for } \alpha,\beta \in Z_2. \tag{1.1}$$

As in the foregoing papers (see Ref. 1, Sec. 2) we denote the degree of a homogeneous element by the "corresponding" lower case Greek letter.

The algebras under consideration will be subalgebras of the general linear Lie superalgebra gl(V,ϵ), with $V = V_{\bar{0}} \oplus V_{\bar{1}}$ a finite-dimensional Z_2-graded vector space. We choose a homogeneous basis $(e_i)_{i\in I}$ in V, i.e., a basis whose members are either even or odd (I is a suitable finite index set). Let $\eta_i \in Z_2$ denote the degree of e_i. It will be convenient to introduce the abbreviations

$$\sigma_i = \epsilon(\eta_i,\eta_i), \quad \sigma_{ij} = \epsilon(\eta_i,\eta_j), \tag{1.2}$$

and

$$d = \mathrm{Tr}_\epsilon(\mathrm{id}_V) = \dim V_{\bar{0}} - \dim V_{\bar{1}} = \sum_{i\in I}\sigma_i. \tag{1.3}$$

The reader who prefers a matrix notation may want to use the basis $(\mathrm{E}_{ij})_{i,j\in I}$ of gl(V,ϵ) which canonically corresponds to $(e_i)_{i\in I}$; by definition, E_{ij} is the linear mapping of V into itself whose matrix with respect to the basis $(e_i)_{i\in I}$ is given by

$$(\mathrm{E}_{ij})_{kl} = \delta_{ik}\delta_{jl}, \quad i,j,k,l \in I. \tag{1.4}$$

In the course of our investigations we have to introduce a total ordering on I. This ordering will be used to define the $I \times I$ matrix (ξ_{ij}) by

$$\xi_{ij} = \begin{cases} 1 & \text{if } i<j \\ 0 & \text{if } i \geqslant j. \end{cases} \tag{1.5}$$

At this point we would like to stress that the meaning of several other symbols, like X_{ij}, h, ϵ_i,..., changes from section to section. These symbols denote objects which are only analogous, namely, the generators of the algebra in question, a Cartan subalgebra, certain basic linear forms on h,... . Our notation would be unnecessarily cumbersome if we wanted to avoid this slight ambiguity. In all cases, the Casimir elements under investigation are then given by

$$C_n = \sum_{i_1,\ldots,i_n \in I} \sigma_{i_1}\sigma_{i_2}\cdots\sigma_{i_{n-1}} X_{i_n i_1} X_{i_1 i_2} \cdots X_{i_{n-1} i_n}, \tag{1.6}$$

where the right-hand side is calculated in the enveloping algebra.

2. THE GENERAL LINEAR LIE SUPERALGEBRAS

We start from the canonical gl(V,ϵ)-invariant bilinear mapping [see Ref. 1, Eq. (6.6)]

$$t\colon\ V \times V^* \to \mathrm{gl}(V,\epsilon) \tag{2.1a}$$

given by

[a)] Supported by the Deutsche Forschungsgemeinschaft.

$$t(y,x')x = x'(x)y \tag{2.1b}$$

for all $x, y \in V$ and $x' \in V^*$. Let $(e_i)_{i\in I}$ be a homogeneous basis of V and let $(e'_j)_{j\in I}$ denote the corresponding dual basis of V^*,

$$e'_j(e_i) = \delta_{ij} \quad \text{for all } i,j\in I. \tag{2.2}$$

We define the generators X_{ij} of $\mathrm{gl}(V,\epsilon)$ by

$$X_{ij} = t(e_i, e'_j) \quad \text{for all } i,j\in I. \tag{2.3}$$

Obviously, we have

$$X_{ij} = E_{ij} \quad \text{for all } i,j\in I. \tag{2.4}$$

Let h denote the subspace of $\mathrm{gl}(V,\epsilon)$ which is generated by the elements X_{ii}, $i\in I$. Of course, h is nothing but the subalgebra of all elements of $\mathrm{gl}(V,\epsilon)$ whose matrix with respect to the basis (e_i) is diagonal.

For every $j\in I$, we define a linear form ϵ_j on h through the equation

$$He_j = \epsilon_j(H)e_j \quad \text{for all } H\in h. \tag{2.5}$$

This implies that

$$\epsilon_j(X_{ii}) = \delta_{ij} \quad \text{for all } i,j\in I. \tag{2.6}$$

Thus, $(\epsilon_j)_{j\in I}$ is the basis of h^* which is dual to the basis $(X_{ii})_{i\in I}$ of h.

The invariance of t implies that

$$\langle H, X_{ij}\rangle = (\epsilon_i - \epsilon_j)(H)X_{ij} \tag{2.7}$$

for all $H\in h$ and all $i,j\in I$. Consequently, h is a Cartan subalgebra of $\mathrm{gl}(V,\epsilon)$,

$$\Delta = \{\epsilon_i - \epsilon_j \,|\, i,j\in I;\ i\neq j\} \tag{2.8}$$

is the root system of $\mathrm{gl}(V,\epsilon)$ with respect to h, and X_{ij} (with $i\neq j$) is a root vector corresponding to $\epsilon_i - \epsilon_j$. Note that the root $\epsilon_i - \epsilon_j$ is even/odd depending on whether $\sigma_i\sigma_j = \pm 1$.

To introduce an adequate bilinear form on h^* we proceed as in the classical case. The invariant bilinear form

$$(X,Y)\to \mathrm{Tr}_\epsilon(XY) \tag{2.9}$$

on $\mathrm{gl}(V,\epsilon)$ is ϵ-symmetric and nondegenerate, consequently, its restriction to h is likewise. Let $(\ |\ )$ denote the bilinear form on h^*, which is inverse to this restriction. We recall its definition. For any $\lambda\in h^*$ there is a unique element $H_\lambda\in h$ such that

$$\lambda(H) = \mathrm{Tr}_\epsilon(H_\lambda H) \quad \text{for all } H\in h. \tag{2.10}$$

Then we define, for all $\lambda,\mu\in h^*$,

$$(\lambda|\mu) = \lambda(H_\mu) = \mu(H_\lambda) = \mathrm{Tr}_\epsilon(H_\lambda H_\mu). \tag{2.11}$$

It is easy to check that

$$H_\lambda = \sum_{i\in I}\sigma_i\lambda(X_{ii})X_{ii} \quad \text{for all } \lambda\in h^* \tag{2.12}$$

and that

$$(\epsilon_i|\epsilon_j) = \sigma_i\delta_{ij} \quad \text{for all } i,j\in I. \tag{2.13}$$

Let us next specify a system of positive roots or, what amounts to the same, a basis of the root system Δ. Choose any total ordering on I. Let $i_1, i_2,\ldots,i_p$ be the strictly increasing sequence of elements of I. We set

$$\bar\epsilon_q = \epsilon_{i_q} \quad \text{if } 1\leqslant q\leqslant p \tag{2.14}$$

and define

$$\alpha_q = \bar\epsilon_q - \bar\epsilon_{q+1} \quad \text{for } 1\leqslant q\leqslant p-1. \tag{2.15}$$

Then $(\alpha_q)_{1<q<p-1}$ is a basis of the subspace of h^* generated by Δ (that is, of $\{\lambda\in h^*|\lambda(\mathrm{id})=0\}$), and any root is a linear combination of the α_q with integral coefficients which are either all positive or else all negative. Thus $(\alpha_q)_{1<q<p-1}$ is a basis of Δ in the usual sense; the corresponding system of positive roots is given by

$$\Delta^+ = \{\epsilon_i - \epsilon_j \,|\, i,j\in I;\ i<j\}, \tag{2.16}$$

and the system of negative roots is $\Delta^- = -\Delta^+$. Conversely, the α_q are the "indecomposable" elements of Δ^+.

For later reference, we define the element $\rho\in h^*$ to be half the sum of the even positive roots minus half the sum of the odd positive roots. It is easy to check that

$$\rho = \sum_{i\in I}\sigma_i r_i\epsilon_i \tag{2.17a}$$

with

$$r_i = \sigma_i\,\rho(X_{ii}) = \frac{1}{2}\Big(\sum_{j>i}\sigma_j - \sum_{j<i}\sigma_j\Big) \tag{2.17b}$$

for all $i\in I$.

The coefficients r_i satisfy some remarkable identities. In fact, it can be shown that for all integers $p\geqslant 0$

$$\sum_{i\in I}\sigma_i r_i^{2p+1} = 0, \tag{2.18}$$

whereas

$$\sum_{q=0}^{p}\binom{2p+1}{2q}\sum_{i\in I}\sigma_i(2r_i)^{2q} = d^{2p+1}. \tag{2.19}$$

By Eq. (2.18), the nonzero $\sigma_i r_i$ come by pairs of opposite sign. On the other hand, Eq. (2.19) implies that the sums $\Sigma_{i\in I}\sigma_i r_i^{2p}$ are (universal) polynomials in d of degree $2p+1$.

Now let Λ be any linear form on h. We use the results of Ref. 2, Sec. 7, to calculate the eigenvalue $\chi_\Lambda(C_n)$ of C_n in a highest weight module with highest weight Λ. The coefficients c_{ij} [see Ref. 2, Eq. (7.9)] are all equal to 1. Consequently, we have

$$\chi_\Lambda(C_n) = \sum_{i,j}(A^n)_{ij}\sigma_j, \tag{2.20}$$

with the $I\times I$ matrix A given by

$$A_{ij} = \Big(\sigma_i\Lambda(X_{ii}) + \sum_k \xi_{ik}\sigma_k\Big)\delta_{ij} - \sigma_i\xi_{ij}. \tag{2.21}$$

A brief calculation shows that

$$\sum_k \xi_{ik}\sigma_k = r_i + \tfrac{1}{2}(d-\sigma_i), \tag{2.22}$$

where r_i has been defined in Eq. (2.17). Thus we obtain

$$A_{ij} = (\sigma_i(\Lambda+\rho)(X_{ii}) + \tfrac{1}{2}(d-\sigma_i))\delta_{ij} - \sigma_i\xi_{ij}. \tag{2.23}$$

It is very welcome that in this way A_{ij} [and hence $\chi_\Lambda(C_n)$] is already written in terms of the variable $\lambda = \Lambda + \rho$ (see Refs. 10 and 11).

To proceed,[8] we introduce the abbreviations

$$l_i = \sigma_i\lambda(X_{ii}), \tag{2.24}$$

$$d_i = l_i + \tfrac{1}{2}(d-\sigma_i), \tag{2.25}$$

and consider the polynomial function c_n of $\lambda\in h^*$ defined by

$$c_n(\lambda) = \chi_\Lambda(C_n) = \sum_{i,j} (A^n)_{ij}\sigma_j. \tag{2.26}$$

The sum can be calculated by diagonalizing the matrix A. We obtain

$$c_n = \sum_{i\in I} \sigma_i a_i d_i^n \tag{2.27a}$$

with

$$a_i = \prod_{j\neq i}\left(1 - \frac{\sigma_j}{d_i - d_j}\right). \tag{2.27b}$$

Remark: At this place, a few comments are in order. The triangular matrix A can be diagonalized if the diagonal elements d_i are all different [see the denominators in Eq. (2.27b)]. On the other hand, we know that c_n is a polynomial function. This implies that if the a_i of Eq. (2.27b) are inserted into Eq. (2.27a), the denominators $d_i - d_j$ must turn out to be spurious, i.e., they must cancel against similar factors in the nominator. In this sense, Eq. (2.27) holds for all $\lambda\in h^*$. A similar remark applies to some of the subsequent formulae.

Now let z be an indeterminate. We introduce the generating function for the c_n by

$$G(z) = \sum_{n\geqslant 0} c_n z^n = \sum_{i\in I}\sigma_i a_i (1 - d_i z)^{-1}. \tag{2.28}$$

(In the following, all "functions" of z are to be interpreted as formal power series in z.) It is not difficult to prove that

$$G(z) = (1/z)(1 - F(z)) \tag{2.29}$$

with

$$F(z) = \prod_{i\in I}\left(1 - \frac{\sigma_i z}{1 - d_i z}\right). \tag{2.30}$$

Introducing the new function $f(z)$ by

$$F(z) = (1 - dz)e^{-f(z)} \tag{2.31}$$

we rewrite Eq. (2.29) as

$$G(z) = (1/z)(1 - e^{-f(z)}) + de^{-f(z)}. \tag{2.32}$$

To calculate $f(z)$, we take logarithms in Eq. (2.31) and obtain

$$f(z) = \sum_{r\geqslant 2}\left(\sum_{s\geqslant 0}\frac{1}{r}\binom{r}{r-1-2s}2^{-2s}R_{r-1-2s}\right)z^r \tag{2.33}$$

with

$$R_p = \sum_{i\in I}\sigma_i\left(\left(l_i + \frac{d}{2}\right)^p - \left(r_i + \frac{d}{2}\right)^p\right). \tag{2.34}$$

Obviously, we have

$$R_p = \sum_{m=0}^{p}\binom{p}{m}\left(\frac{d}{2}\right)^{p-m}Q_m, \tag{2.35}$$

where

$$Q_m = \sum_{i\in I}\sigma_i(l_i^m - r_i^m). \tag{2.36}$$

We prefer to work with the functions Q_m instead of the R_p. According to the above results, the functions c_n can be written as polynomials in the Q_m.

The Q_m are polynomial functions of λ. We notice that they are invariant under the transformation $l_i \to l_{\tau(i)}$, where τ is any permutation of I which satisfies $\sigma_{\tau(i)} = \sigma_i$ for all $i\in I$. This is exactly the invariance under the Weyl group of $\mathrm{gl}(V,\epsilon)$. Consequently, the functions c_n are Weyl-invariant as well.[10,11] We stress that this is not at all obvious from Eq. (2.20).

Using the above formulae, we obtain the following expressions for the functions c_n in terms of the Q_m:

$$\begin{aligned}
&c_0 = d, \quad c_1 = Q_1, \quad c_2 = Q_2,\\
&c_3 = Q_3 + \tfrac{1}{2}dQ_2 - \tfrac{1}{2}Q_1^2 - \tfrac{1}{4}(d^2-1)Q_1,\\
&c_4 = Q_4 + dQ_3 - Q_1Q_2 + \tfrac{1}{2}Q_2 - \tfrac{1}{2}dQ_1^2 - \tfrac{1}{4}d(d^2-1)Q_1,\\
&c_5 = Q_5 + \tfrac{3}{2}dQ_4 - \tfrac{1}{2}Q_2^2 - Q_1Q_3 + \tfrac{1}{6}(3d^2+5)Q_3\\
&\quad - \tfrac{3}{2}dQ_1Q_2 + \tfrac{1}{6}Q_1^3 - \tfrac{1}{4}d(d^2-3)Q_2 - \tfrac{1}{4}(d^2+1)Q_1^2\\
&\quad - \tfrac{1}{16}(d^2-1)(3d^2+1)Q_1.
\end{aligned} \tag{2.37}$$

These relations have also been derived directly from Eq. (2.20). We note that $c_n - Q_n$ has degree $\leqslant n-1$, for all integers $n\geqslant 1$.

In closing this section we recall that the bilinear form (2.9) provides us with a quadratic Casimir element C_2' (see the example in Sec. 4 of Ref. 2). Actually, a brief calculation shows that $C_2' = C_2$. On the other hand, it is well known[4] that the eigenvalue of C_2' in a highest weight module with highest weight Λ is equal to $(\Lambda\,|\Lambda + 2\rho)$. This result agrees with Eq. (2.37).

3. THE SPECIAL LINEAR LIE SUPERALGEBRAS

This case is completely analogous to the foregoing one; however, we have to *assume that d is different from zero.*

According to Ref. 1, Sec. 8 the bilinear mapping

$$t:\ V\times V^* \to \mathrm{sl}(V,\epsilon), \tag{3.1a}$$

defined by

$$t(y,x')x = x'(x)y - (1/d)\epsilon(\eta,\xi')x'(y)x \tag{3.1b}$$

for all homogeneous elements $x, y\in V$ and $x'\in V^*$, is $\mathrm{gl}(V,\epsilon)$-invariant, and its image generates the vector space $\mathrm{sl}(V,\epsilon)$. As before, let $(e_i)_{i\in I}$ be a homogeneous basis of V, and let $(e_j')_{j\in I}$ denote the corresponding dual basis of V^*. We define the generators X_{ij} of $\mathrm{sl}(V,\epsilon)$ by

$$X_{ij} = t(e_i, e_j') \quad \text{for all } i,j\in I. \tag{3.2}$$

Obviously, we have

$$X_{ij} = E_{ij} - (1/d)\sigma_i\delta_{ij}\mathrm{id} \quad \text{for all } i,j\in I. \tag{3.3}$$

Let h denote the subspace of $\mathrm{sl}(V,\epsilon)$ which is generated by the elements X_{ii}, $i\in I$. Of course, h is nothing but the subalgebra of all elements of $\mathrm{sl}(V,\epsilon)$ whose matrix with respect to the basis (e_i) is diagonal. Note that

$$\sum_{i\in I} X_{ii} = 0. \tag{3.4}$$

For every $j\in I$, we define a linear form ϵ_j on h through the equation

$$He_j = \epsilon_j(H)e_j \quad \text{for all } H\in h. \tag{3.5}$$

It follows that

$$\epsilon_j(X_{ii}) = \delta_{ij} - (1/d)\sigma_i \quad \text{for all } i,j\in I. \tag{3.6}$$

In particular, the $\epsilon_j, j\in I$, generate the vector space h^*, and we have

$$\sum_{j\in I}\sigma_j\epsilon_j = 0. \tag{3.7}$$

The invariance of t implies that

$$\langle H, X_{ij}\rangle = (\epsilon_i - \epsilon_j)(H)X_{ij} \tag{3.8}$$

for all $H\in h$ and all $i,j\in I$. Consequently, h is a Cartan subalgebra of $\mathrm{sl}(V,\epsilon)$,

$$\Delta = \{\epsilon_i - \epsilon_j \mid i,j\in I;\ i\neq j\} \tag{3.9}$$

is the root system of $\mathrm{sl}(V,\epsilon)$ with respect to h, and X_{ij} (with $i\neq j$) is a root vector corresponding to $\epsilon_i - \epsilon_j$. Once again, the root $\epsilon_i - \epsilon_j$ is even/odd depending on whether $\sigma_i\sigma_j = \pm 1$.

To introduce an adequate bilinear form on h^* we recall (see Ref. 1, Sec. 8) that the invariant bilinear form

$$(X,Y)\rightarrow \mathrm{Tr}_\epsilon(XY) \tag{3.10}$$

on $\mathrm{sl}(V,\epsilon)$ is ϵ-symmetric and nondegenerate; consequently, its restriction to h is likewise. Let $(\ |\ )$ denote the bilinear form on h^*, which is inverse to this restriction; by definition, we have

$$(\lambda|\mu) = \mathrm{Tr}_\epsilon(H_\lambda H_\mu) \tag{3.11}$$

for all $\lambda,\mu\in h^*$, where, for example, the element $H_\lambda\in h$ is uniquely defined through the equation

$$\lambda(H) = \mathrm{Tr}_\epsilon(H_\lambda H) \quad \text{for all } H\in h. \tag{3.12}$$

It is easy to check that

$$H_\lambda = \sum_{i\in I}\sigma_i\lambda(X_{ii})X_{ii} \quad \text{for all } \lambda\in h^* \tag{3.13}$$

and that

$$(\epsilon_i|\epsilon_j) = \sigma_i\delta_{ij} - 1/d \quad \text{for all } i,j\in I. \tag{3.14}$$

We shall next specify a system of positive roots, that is, a basis of the root system Δ. Choose any total ordering on I and let $i_1,i_2,...,i_p$ be the strictly increasing sequence of elements of I. We set

$$\bar\epsilon_q = \epsilon_{i_q} \quad \text{if } 1\leqslant q\leqslant p \tag{3.15}$$

and define

$$\alpha_q = \bar\epsilon_q - \bar\epsilon_{q+1} \quad \text{for } 1\leqslant q\leqslant p-1. \tag{3.16}$$

Then $(\alpha_q)_{1\leqslant q\leqslant p-1}$ is a basis of h^*, and any root is a linear combination of the α_q with integral coefficients which are either all positive or else all negative. Thus $(\alpha_q)_{1\leqslant q\leqslant p-1}$ is a basis of Δ in the usual sense, the corresponding system of positive roots is given by

$$\Delta^+ = \{\epsilon_i - \epsilon_j \mid i,j\in I;\ i<j\}, \tag{3.17}$$

and the system of negative roots is $\Delta^- = -\Delta^+$. Conversely, the α_q are the "indecomposable" elements of Δ^+.

Consider next the element $\rho\in h^*$, which is defined to be half the sum of the even positive roots minus half the sum of the odd positive roots. As before, we have

$$\rho = \sum_{i\in I}\sigma_i r_i\epsilon_i \tag{3.18a}$$

with

$$r_i = \sigma_i\rho(X_{ii}) = \frac{1}{2}\Big(\sum_{j>i}\sigma_j - \sum_{j<i}\sigma_j\Big) \tag{3.18b}$$

for all $i\in I$. Note that the coefficients r_i are *the same* as those for $\mathrm{gl}(V,\epsilon)$ [see Eq. (2.17)]; in particular, the relations (2.18), (2.19) are again satisfied.

Remark: Of course, the foregoing formulae are closely related to the analogous ones for $\mathrm{gl}(V,\epsilon)$. To establish the connection, let us keep the notation of the $\mathrm{gl}(V,\epsilon)$ case, but let us mark the entries corresponding to $\mathrm{sl}(V,\epsilon)$ by a superscript s. The relation between the generators X_{ij} and X^s_{ij} can be read off from Eqs. (2.4) and (3.3). In particular, h^s is the subspace of all ϵ-traceless elements of h and ϵ^s_j is the restriction of ϵ_j onto h^s. Quite generally, let λ^s denote the restriction of λ to h^s, for all $\lambda\in h^*$. Then the mapping $\lambda\rightarrow\lambda^s$ is a vector space isomorphism of $h' = \{\lambda\in h^* \mid \lambda(\mathrm{id}) = 0\}$ onto $(h^s)^*$, which is compatible with the bilinear forms (2.11) and (3.11). If we identify h' and $(h^s)^*$ by means of this isomorphism, the root systems of $\mathrm{gl}(V,\epsilon)$ and $\mathrm{sl}(V,\epsilon)$ (with respect to h and h^s, respectively) are just the same.

After this interruption, we return to our earlier notation (without the superscript s) and resume the general discussion. Let Λ be any linear form on h. We apply the results of Ref. 2, Sec. 7, and calculate the eigenvalue $\chi_\Lambda(C_n)$ of C_n in a highest weight module with highest weight Λ. The coefficients c_{ij} [see Ref. 2, Eq. (7.9)] are given by

$$c_{ij} = 1 - (1/d)\sigma_i\delta_{ij} \quad \text{for all } i,j\in I. \tag{3.19}$$

Using the relation (2.22), we thus obtain

$$\chi_\Lambda(C_n) = c_n(\Lambda + \rho), \tag{3.20}$$

where

$$c_n(\lambda) = \sum_{i,j}(A^n)_{ij}\sigma_j, \tag{3.21}$$

and where the $I\times I$ matrix A is given by

$$A_{ij} = (\sigma_i\lambda(X_{ii}) + \tfrac{1}{2}(d-\sigma_i))\delta_{ij} - \sigma_i\xi_{ij}, \tag{3.22}$$

for all $\lambda\in h^*$.

These formulae are completely analogous to those for $\mathrm{gl}(V,\epsilon)$. In fact, if we use the identification described in the previous remark, the function c_n for $\mathrm{sl}(V,\epsilon)$ is just the function c_n for $\mathrm{gl}(V,\epsilon)$ restricted to h'. Consequently, the evaluation of the formulae for $\mathrm{gl}(V,\epsilon)$ applies to the algebra $\mathrm{sl}(V,\epsilon)$ as well. Actually, the results simplify considerably, for in the present case we have $R_1 = Q_1 = 0$.

We close this section by two remarks. First we recall that the bilinear form (3.10) provides us with a quadratic Casimir element C_2' (see the example in Sec. 4 of Ref. 2). Once again, we have $C_2' = C_2$, and the eigenvalue of C_2' in a highest weight module with highest weight Λ is equal to $(\Lambda|\Lambda + 2\rho)$.

As a second remark, we note that the discussion of the present and the foregoing section applies to all (finite-dimensional) Γ-graded vector spaces V, with Γ an arbitrary abelian group of degrees, and to all commutation factors ϵ. This will no longer be true for the orthosymplectic algebras, which we are going to investigate in the subsequent section (see the example in Sec. 10 A of Ref. 1).

4. THE ORTHOSYMPLECTIC LIE SUPERALGEBRAS

Let b be a nondegenerate even ϵ-symmetric bilinear form on V. Stated differently, this means that $V_{\bar 0}$ and $V_{\bar 1}$ are orthogonal with respect to b and that the restriction of b onto $V_{\bar{0}}$ (resp. onto $V_{\bar{1}}$) is nondegenerate and symmetric (resp. skew-symmetric). It follows that dim $V_{\bar{1}}$ is even.

We are going to investigate the orthosymplectic Lie superalgebra osp (b). In doing so we assume that the following conditions are satisfied:

(a) The Witt index ν of the restriction of b onto $V_{\bar{0}}$ is maximal, that is, dim $V_{\bar{0}}$ is equal to 2ν or $2\nu + 1$, depending on whether it is even or odd.

(b) The discriminant of b has the form $(-1)^\nu a^2$ with some nonzero element a of K.

Condition (a) is crucial, it ensures that the reductive Lie algebra osp $(b)_{\bar{0}}$ has a splitting Cartan subalgebra. On the other hand, condition (b) is made only for convenience. In fact, because of (a) it is always satisfied if dim $V_{\bar{0}}$ is even, and it is fulfilled for suitable nonzero scalar multiples of b if dim $V_{\bar{0}}$ is odd. (Recall that all nonzero scalar multiples of b yield the same orthosymplectic Lie superalgebra.) Both conditions are automatically satisfied if the base field is algebraically closed.

Remark: The conditions (a) and (b) are fulfilled if and only if there exists a homogeneous basis $(e_i)_{i \in I}$ of V such that the relations (4.1) hold. Consequently, the reader who is not acquainted with the notions of Witt index and discriminant may replace these conditions by the requirement that such a basis does exist.

In the following we want to treat all possible cases simultaneously. This requires a careful choice of notation. Let I denote an index set containing exactly dim V elements. We choose a permutation π of I with $\pi^2 = \mathrm{id}$ such that π has no fixed point if dim $V_{\bar{0}}$ is even and exactly one fixed point, called o, if dim $V_{\bar{0}}$ is odd. Furthermore, let J be a subset of I such that I is the disjoint union of J and $\pi(J)$ if dim $V_{\bar{0}}$ is even and the disjoint union of J, $\pi(J)$, and $\{o\}$ if dim $V_{\bar{0}}$ is odd.

According to our conditions (a) and (b) there exists a homogeneous basis $(e_i)_{i \in I}$ of V such that

$$b(e_i, e_j) = 0 \quad \text{if } i, j \in I \text{ and } \pi(j) \neq i, \tag{4.1a}$$

$$b(e_{\pi(j)}, e_j) = 1 \quad \text{if } j \in J, \tag{4.1b}$$

and

$$b(e_o, e_o) = 1 \quad \text{if dim } V_{\bar{0}} \text{ is odd.} \tag{4.1c}$$

Recall that the degree of e_i is denoted by η_i and that $\sigma_i = \epsilon(\eta_i, \eta_i)$. The relations (4.1) imply that

$$\eta_{\pi(i)} = \eta_i \quad \text{for all } i \in I \tag{4.2a}$$

and

$$\eta_o = \bar{0} \quad \text{if dim } V_{\bar{0}} \text{ is odd,} \tag{4.2b}$$

that is to say,

$$\sigma_{\pi(i)} = \sigma_i \quad \text{for all } i \in I \tag{4.3a}$$

and

$$\sigma_o = 1 \quad \text{if dim } V_{\bar{0}} \text{ is odd.} \tag{4.3b}$$

We set for both $\alpha \in Z_2$

$$I_\alpha = \{ i \in I \mid \eta_i = \alpha \} \tag{4.4}$$

and

$$J_\alpha = J \cap I_\alpha. \tag{4.5}$$

Finally, let us introduce the basis $(f_j)_{j \in I}$ of V which is dual to $(e_i)_{i \in I}$ with respect to b, in the sense that

$$b(f_j, e_i) = \delta_{ij} \quad \text{for all } i, j \in I. \tag{4.6}$$

According to the relations (4.1), we have

$$f_i = \tau_i e_{\pi(i)} \quad \text{for all } i \in I, \tag{4.7}$$

where

$$\tau_j = 1 \quad \text{and} \quad \tau_{\pi(j)} = \sigma_j \quad \text{for all } j \in J \tag{4.8a}$$

and

$$\tau_o = 1 \quad \text{if dim } V_{\bar{0}} \text{ is odd.} \tag{4.8b}$$

Note that

$$\tau_i \tau_{\pi(i)} = \sigma_i \quad \text{for all } i \in I. \tag{4.9}$$

After these preliminaries we may now proceed to investigate the orthosymplectic Lie superalgebra osp(b). We start from the canonical bilinear mapping [see Ref. 1, Eq. (10.13)]

$$t: \; V \times V \to \mathrm{osp}(b) \tag{4.10a}$$

given by

$$t(x, y)z = b(y, z)x - \epsilon(\xi, \eta) b(x, z) y \tag{4.10b}$$

for all homogeneous elements $x, y, z \in V$. Recall that t is ϵ-skew-symmetric even and osp(b)-invariant and that its image generates the vector space osp(b).

Using the bases introduced above we define the generators X_{ij} of osp(b) by

$$X_{ij} = t(e_i, f_j) \quad \text{for all } i, j \in I. \tag{4.11}$$

We note that X_{ij} is homogeneous of degree $\eta_i + \eta_j$ and that

$$X_{ij} = -\sigma_{ij} \tau_{\pi(i)} \tau_j X_{\pi(j), \pi(i)} \quad \text{for all } i, j \in I \tag{4.12}$$

[recall Eq. (1.2)], which implies

$$X_{i, \pi(i)} = 0 \quad \text{if } i \in I_{\bar{0}}. \tag{4.13}$$

A brief calculation shows that

$$X_{ij} = E_{ij} - \sigma_{ij} \tau_{\pi(i)} \tau_j E_{\pi(j), \pi(i)} \tag{4.14}$$

for all $i, j \in I$.

Remark: Of course, we could also work with the generators $t(e_i, e_j)$ which satisfy a simpler symmetry relation.

Now let h denote the subspace of osp(b) which is generated by the elements X_{ii}, $i \in I$. Evidently, h is nothing but the subalgebra of all elements of osp(b) whose matrix with respect to the basis (e_i) is diagonal. Since

$$X_{ii} = -X_{\pi(i), \pi(i)} \quad \text{for all } i \in I, \tag{4.15}$$

the vector space h is already generated by the elements X_{jj} with $j \in J$.

For every $i \in I$ we define a linear form ϵ_i on h through the equation

$$H e_i = \epsilon_i(H) e_i \quad \text{for all } H \in h. \tag{4.16}$$

Then it is not difficult to see that

$$\epsilon_{\pi(i)} = -\epsilon_i \quad \text{for all } i \in I \tag{4.17}$$

(in particular, $\epsilon_o = 0$ if dim $V_{\bar{0}}$ is odd) and that

$$\epsilon_i(X_{jj}) = \delta_{ij} \quad \text{for all } i, j \in J. \tag{4.18}$$

Consequently, $(X_{jj})_{j \in J}$ is a basis of h and $(\epsilon_j)_{j \in J}$ is the corresponding dual basis of h^*.

The invariance of t implies that

$$\langle H, X_{ij}\rangle = (\epsilon_i - \epsilon_j)(H)X_{ij} \tag{4.19}$$

for all $H\in h$ and $i,j\in I$. Note that $\epsilon_i - \epsilon_j$ is equal to zero if and only if $j = i$, in which case X_{ij} is an element of h. On the other hand, X_{ij} is equal to zero if and only if $j = \pi(i)\in I_{\bar 0}$. Consequently, h is a Cartan subalgebra of osp(b),

$$\Delta = \{\epsilon_i - \epsilon_j | i,j\in I; j\neq i,\pi(i) \text{ or } j = \pi(i)\in I_{\bar 1}\} \tag{4.20}$$

is the root system of osp(b) with respect to h, and X_{ij} [with i,j as specified in Eq. (4.20)] is a root vector corresponding to $\epsilon_i - \epsilon_j$. The root $\epsilon_i - \epsilon_j$ is even/odd depending on whether $\sigma_i\sigma_j = \pm 1$.

To introduce an adequate bilinear form on h^*, we recall that the invariant bilinear form

$$(X,Y)\rightarrow \tfrac{1}{2}\,\mathrm{Tr}_\epsilon(XY) \tag{4.21}$$

on osp(b) is ϵ-symmetric and nondegenerate; consequently, its restriction to h is likewise. Let $(\ |\ )$ denote the bilinear form on h^*, which is inverse to this restriction; by definition, we have

$$(\lambda|\mu) = \tfrac{1}{2}\,\mathrm{Tr}_\epsilon(H_\lambda H_\mu) \tag{4.22}$$

for all $\lambda,\mu\in h^*$, where, for example, the element $H_\lambda\in h$ is uniquely defined through the equation

$$\lambda(H) = \tfrac{1}{2}\,\mathrm{Tr}_\epsilon(H_\lambda H) \quad \text{for all } H\in h. \tag{4.23}$$

It is easy to check that

$$H_\lambda = \sum_{j\in J}\sigma_j\lambda(X_{jj})X_{jj} \quad \text{for all } \lambda\in h^* \tag{4.24}$$

and that

$$(\epsilon_i|\epsilon_j) = \sigma_i\delta_{ij} \quad \text{for all } i,j\in J. \tag{4.25}$$

Let us next specify a system of positive roots or, what amounts to the same, a basis of the root system Δ. If $\dim V\leqslant 1$, or if $\dim V = 2$ and $V = V_{\bar 0}$, then Δ is empty, and we are done. Otherwise, choose any total ordering on J and let $j_1, j_2,\ldots,j_p$ be the strictly increasing sequence of elements of J. We set

$$\bar\epsilon_q = \epsilon_{j_q} \quad \text{for } 1\leqslant q\leqslant p \tag{4.26}$$

and define

$$\alpha_q = \bar\epsilon_q - \bar\epsilon_{q+1} \quad \text{if } 1\leqslant q\leqslant p-1, \tag{4.27a}$$

$$\alpha_p = \begin{cases}\bar\epsilon_p & \text{if } \dim V_{\bar 0} \text{ is odd,}\\ \bar\epsilon_{p-1} + \bar\epsilon_p & \text{if } \dim V_{\bar 0} \text{ is even and } j_p\in J_{\bar 0},\\ 2\bar\epsilon_p & \text{if } \dim V_{\bar 0} \text{ is even and } j_p\in J_{\bar 1}.\end{cases} \tag{4.27b}$$

Then $(\alpha_q)_{1\leqslant q\leqslant p}$ is a basis of h^*, and any root is a linear combination of the α_q with integral coefficients which are either all positive or else all negative. Thus $(\alpha_q)_{1\leqslant q\leqslant p}$ is a basis of Δ in the usual sense, and the corresponding positive roots are the following:

$\epsilon_i - \epsilon_j$ with $i,j\in J$, $i<j$,
$\epsilon_i + \epsilon_j$ with $i,j\in J$, $i<j$,
$2\epsilon_j$ with $j\in J_{\bar 1}$,

and in addition, if $\dim V_{\bar 0}$ is odd,

ϵ_j with $j\in J$.

As before, the system of positive roots is denoted by Δ^+ and the system of negative roots is $\Delta^- = -\Delta^+$. We note that the α_q are the "indecomposable" elements of Δ^+.

The above description of the positive roots works also for the degenerate cases which had been excluded. In fact, in these cases J has a unique (total) ordering, and our prescription yields the empty subset of h^*, as it should.

Now let $\rho\in h^*$ be half the sum of the even positive roots minus half the sum of the odd positive roots. Then it is not difficult to check that

$$\rho = \sum_{j\in J}\sigma_j r_j\epsilon_j, \tag{4.28a}$$

with

$$r_j = \sum_{\substack{i\in J\\ i>j}}\sigma_i + \tfrac{1}{2}(\sigma_j - 1 + \omega) \tag{4.28b}$$

for all $j\in J$ and

$$\omega = \begin{cases}0 & \text{if } \dim V_{\bar 0} \text{ is even}\\ 1 & \text{if } \dim V_{\bar 0} \text{ is odd.}\end{cases} \tag{4.29}$$

The coefficients r_j satisfy the relations

$$\sum_{q=1}^{p}\binom{2p+1}{2q}2\sum_{j\in J}\sigma_j(2r_j)^{2q} = (d-1)^{2p+1} - (d-1), \tag{4.30}$$

for all integers $p\geqslant 1$. Consequently, the sums $\Sigma_{j\in J}\sigma_j r_j^{2p}$ are (universal) polynomials in d of degree $2p+1$.

It will turn out convenient to extend the definition of the r_i to all indices $i\in I$ by the requirement that

$$r_{\pi(i)} = -r_i \quad \text{for all } i\in I. \tag{4.31}$$

Then we have

$$r_i = \sigma_i\,\rho(X_{ii}) \quad \text{for all } i\in I. \tag{4.32}$$

In view of the subsequent discussion, let us next extend the given ordering on J to a total ordering of I. This extension is uniquely fixed by the requirement that the following relations should be satisfied for all $i,j\in J$:

$$\pi(i) < \pi(j) \quad \text{if and only if} \quad j<i, \tag{4.33}$$

$$i<\pi(j), \tag{4.34a}$$

$$i<o<\pi(j) \quad \text{if } \dim V_{\bar 0} \text{ is odd.} \tag{4.34b}$$

Obviously, the relation (4.33) then holds for all $i,j\in I$.

Now let Λ be any linear form on h. We use the results of Ref. 2, Sec. 7, to calculate the eigenvalue $\chi_\Lambda(C_n)$ of C_n in a highest weight module with highest weight Λ. The coefficients c_{ij} [see Ref. 2, Eq. (7.9)] are given by

$$c_{ij} = 1 - \sigma_i\delta_{i,\pi(j)} \quad \text{for all } i,j\in I. \tag{4.35}$$

Furthermore, a brief discussion shows that for all indices $i,j\in I$ with $i<j$, the linear form $\Lambda + (\epsilon_i - \epsilon_j)$ is not a weight of the given module (note that this must also be checked in the case $i = \pi(j)\in J_{\bar 0}$). Consequently, we obtain

$$\chi_\Lambda(C_n) = \sum_{i,j\in I}(A^n)_{ij}\sigma_j \tag{4.36}$$

with the $I\times I$ matrix A given by

$$A_{ij} = \Big(\sigma_i\Lambda(X_{ii}) + \sum_{k\in I}\xi_{ik}c_{ik}\sigma_k\Big)\delta_{ij} - \sigma_i\xi_{ij}c_{ij}. \tag{4.37}$$

It is easy to see that for all $i\in I$

$$\sum_{k\in I}\xi_{ik}c_{ik}\sigma_k = r_i + \tfrac{1}{2}(d-\sigma_i - 1 + \delta_{i,\pi(i)}), \tag{4.38}$$

where r_i has been introduced in Eqs. (4.28) and (4.31). Thus we obtain

$$A_{ij} = (\sigma_i\lambda(X_{ii}) + \tfrac{1}{2}(d-\sigma_i - 1 + \delta_{i,\pi(i)}))\delta_{ij} - \sigma_i\xi_{ij}c_{ij}, \tag{4.39}$$

where we have introduced the new variable $\lambda = \Lambda + \rho$.

Now we proceed as in the gl(V,ϵ) case.[8] We use the abbreviations

$$l_i = \sigma_i\lambda(X_{ii}), \tag{4.40}$$

$$d_i = l_i + \tfrac{1}{2}(d-\sigma_i - 1 + \delta_{i,\pi(i)}) \tag{4.41}$$

and consider the polynomial function c_n of $\lambda\in h^*$ defined by

$$c_n(\lambda) = \chi_\Lambda(C_n) = \sum_{i,j\in I}(A^n)_{ij}\sigma_j. \tag{4.42}$$

The sum can be evaluated by diagonalizing the matrix A. After a lengthy calculation we obtain

$$c_n = \sum_{i\in I}\sigma_i a_i d_i^n \tag{4.43a}$$

with

$$a_i = \left(1 - \frac{\sigma_i \pm 1}{d_i - d_{\pi(i)}}\right)\prod_j\left(1 - \frac{\sigma_j}{d_i - d_j}\right) \tag{4.43b}$$

if $i\in J\cup\pi(J)$ and

$$a_o = 1 \quad \text{if } \dim V_{\bar 0} \text{ is odd}. \tag{4.43c}$$

In Eq. (4.43b) the upper/lower sign corresponds to the case where $\dim V_{\bar 0}$ is odd/even, and the product extends over all $j\in I$, which are different from $i,\pi(i)$ and (if $\dim V_{\bar 0}$ is odd) from o. The equations are to be interpreted in the sense of the remark following Eq. (2.27).

Now let z be an indeterminate. We introduce the generating function for the c_n by

$$G(z) = \sum_{n\geqslant 0}c_n z^n = \sum_{i\in I}\sigma_i a_i(1-d_i z)^{-1}. \tag{4.44}$$

(In the following, all "functions" of z are to be interpreted as formal power series in z.) It is not difficult to prove that

$$G(z) = \left(1 + \frac{z}{2-(d-1)z}\right)\frac{1}{z}(1 - F(z)) \tag{4.45}$$

with

$$F(z) = \prod_{i\in I}\left(1 - \frac{\sigma_i z}{1 - d_i' z}\right) \tag{4.46a}$$

and

$$d_i' = d_i - \tfrac{1}{2}\delta_{i,\pi(i)} \quad \text{for all } i\in I. \tag{4.46b}$$

Next we note that

$$d_o = \tfrac{1}{2}(d-1) \tag{4.47}$$

provided $\dim V_{\bar 0}$ is odd. If $\dim V_{\bar 0}$ is even, we consider this equation as a definition for d_o.

Now let x be a new indeterminate. We make a change of variable and introduce the new function $G_0(x)$ by

$$G_0(x) = \frac{1}{1+d_o x}G\left(\frac{x}{1+d_o x}\right), \tag{4.48}$$

the converse equation being

$$G(z) = \frac{1}{1-d_o z}G_0\left(\frac{z}{1-d_o z}\right). \tag{4.49}$$

It follows that

$$G_0(x) = (1 + x/2)(1/x)(1 - F_0(x)) \tag{4.50}$$

with

$$F_0(x) = F\left(\frac{x}{1+d_o x}\right) = \prod_{i\in I}\frac{1-(l_i + \sigma_i/2)x}{1-(l_i - \sigma_i/2)x}. \tag{4.51}$$

Introducing the new function $f(x)$ by

$$F_0(x) = \frac{(1-d_o x)(1-x/2)}{(1+d_o x)(1+x/2)}e^{-f(x)} \tag{4.52}$$

we rewrite equation (4.50) as

$$G_0(x) = \left(1 + \frac{x}{2}\right)\frac{1}{x}(1 - e^{-f(x)}) + \frac{d}{1+d_o x}e^{-f(x)}. \tag{4.53}$$

To calculate $f(x)$, we take logarithms in Eq. (4.51) and obtain

$$f(x) = \sum_{r\geqslant 1}\left(\sum_{s=1}^{r}\frac{1}{2r+1}\binom{2r+1}{2s}2^{1-2(r-s)}Q_{2s}\right)x^{2r+1}, \tag{4.54}$$

where

$$Q_m = \sum_{j\in J}\sigma_j(l_j^m - r_j^m) \tag{4.55}$$

for all integers $m\geqslant 0$.

For practical purposes it is convenient to define the polynomial functions g_r, $r\geqslant 0$, by

$$\frac{1}{x}(1 - e^{-f(x)}) = \sum_{r\geqslant 0}g_r x^r. \tag{4.56}$$

Then Eqs. (4.49) and (4.53) imply that $c_0 = d$ and

$$c_n = g_n + \sum_{r=1}^{n-1}\gamma_{nr}\,g_r \quad \text{if } n\geqslant 1, \tag{4.57}$$

with

$$\gamma_{nr} = \left(\binom{n-1}{r-1} - \binom{n-1}{r}\right)d_o^{n-r} - \frac{1}{2}\left(\binom{n-1}{r} - \binom{n-1}{r+1}\right)d_o^{n-r-1} \tag{4.58}$$

for $1\leqslant r\leqslant n-1$.

According to the above results, the functions c_n can be written as polynomials in the Q_{2m}. The Q_{2m} are polynomial functions of λ. We note that they depend on the l_j^2 only, and that they are invariant under the transformation $l_j \rightarrow l_{\tau(j)}$, where τ is any permutation of J which satisfies $\sigma_{\tau(j)} = \sigma_j$ for all $j\in J$. In particular, the Q_{2m}, and hence also the c_n, are invariant under the Weyl group of osp(b).

Using the above formulae, we obtain the following expressions for the functions c_n in the terms of the Q_{2m}:

$$\begin{aligned}
&c_0 = d, \quad c_1 = 0, \quad c_2 = 2Q_2,\\
&c_3 = (d-2)Q_2, \quad c_4 = 2Q_4 - (d-2)Q_2,\\
&c_5 = (3d-4)Q_4 - 2Q_2^2 - \tfrac{1}{2}(d-2)(d^2-2)Q_2,\\
&c_6 = 2Q_6 + \tfrac{1}{2}(5d^2 - 14d + 14)Q_4\\
&\qquad - (4d-5)Q_2^2 - \tfrac{1}{8}(d-2)(5d^3 - 10d^2 + 8)Q_2.
\end{aligned} \tag{4.59}$$

Once again, these relations have also been derived directly from Eq. (4.42). We note that $c_{2m} - 2Q_{2m}$ has degree $\leqslant 2m-2$, for all integers $m \geqslant 1$.

In closing this section we recall that the bilinear form (4.21) provides us with a quadratic Casimir element C_2' (see the example in Sec. 4 of Ref. 2). It is not difficult to show that $C_2' = \frac{1}{2}C_2$ and that the eigenvalue of C_2' in a highest weight module with highest weight Λ is equal to $(\Lambda \mid \Lambda + 2\rho)$. Furthermore, we note that the results of the present section can be used to establish an isomorphic correspondence between the Casimir elements of the Lie superalgebra $\mathrm{osp}(1,2r)$ and those of the Lie algebra $\mathrm{o}(2r+1)$ such that associated Casimir elements have the same eigenvalue in highest weight modules with the "same" highest weight.[12]

5. AN EXAMPLE: THE ALGEBRA spl(2,1)

The results of the foregoing sections look quite similar to those for the classical Lie algebras. Nevertheless, there are some peculiarities to which we would like to draw the reader's attention.

Consider the algebra $\mathrm{spl}(2,1)$ [that is, $\mathrm{sl}(V,\epsilon)$ with $\dim V_{\bar{0}} = 2$ and $\dim V_{\bar{1}} = 1$]. We keep the notation introduced in section 3. Choose $I = \{1,2,3\}$, endowed with its natural ordering, and assume that

$$\sigma_1 = \sigma_2 = -\sigma_3 = 1. \tag{5.1}$$

It follows that $d = 1$ and

$$r_1 = 0, \quad r_2 = r_3 = -1. \tag{5.2}$$

Now let C be an arbitrary Casimir element of $\mathrm{spl}(2,1)$, that is, an element of $Z(\mathrm{spl}(2,1))$ (see Sec. 4 of Ref. 2). For any $\Lambda \in h^*$ let $\chi_\Lambda(C)$ denote the eigenvalue of C in a highest weight module with highest weight Λ. As before, we set $\lambda = \Lambda + \rho$ and define the polynomial function c on h^* by

$$c(\lambda) = \chi_\Lambda(C). \tag{5.3}$$

The function c can be expressed as a polynomial in the three variables $l_i = \sigma_i \lambda(X_{ii})$, which satisfy the constraint

$$l_1 + l_2 - l_3 = 0. \tag{5.4}$$

In the following we choose l_1, l_2 to be the basic independent variables. Then we deduce from Proposition 2.6 of Ref. 11 that c fulfills the following conditions:

(a) The function c is symmetric in l_1, l_2 (invariance under the Weyl group).

(b) If $i \in \{1,2\}$ and if in c we set $l_i = l_3$, then the resulting polynomial does not depend on the variable $l_i = l_3$.

In view of the constraint (5.4), condition (b) can be rephrased as follows:

(b′) If $j \in \{1,2\}$ and if in c we set $l_j = 0$, then the resulting polynomial is constant.

Let T denote the algebra of all polynomials in l_1, l_2, which satisfy these conditions. It is easy to see that T consists of the polynomials of the form $a + l_1 l_2 P$, with $a \in K$ and P a symmetric polynomial in l_1, l_2.

Of course, the c_n and the Q_m belong to T. Moreover, it is not difficult to prove that 1 and the c_n, $n \geqslant 1$, that is, 1 and the Q_m, $m \geqslant 1$, generate the algebra T. In view of the properties of the Harish–Chandra homomorphism (see Sec. 5 of Ref. 2) this implies that the mapping, which associates with any Casimir element C the polynomial function $\lambda \to \chi_{\lambda-\rho}(C)$ on h^*, is an *isomorphism* of the algebra $Z(\mathrm{spl}(2,1))$ onto the algebra T.

The isomorphism above provides us with a clear picture of the algebra $Z(\mathrm{spl}(2,1))$. First of all, we conclude that 1 and the Casimir elements C_n, $n \geqslant 2$, generate this algebra. Stated differently, any Casimir element of $\mathrm{spl}(2,1)$ can be written as a polynomial in the C_n, $n \geqslant 2$. A brief discussion shows that no proper subfamily of $(C_n)_{n\geqslant 2}$ has this property. Moreover, it is easy to see that no finite subset generates the algebra $Z(\mathrm{spl}(2,1))$. Of course, this does not mean that the C_n are algebraically independent. On the contrary, any three elements of $Z(\mathrm{spl}(2,1))$ are algebraically dependent.

In spite of the fact that C_2 and C_3 do not generate the algebra $Z(\mathrm{spl}(2,1))$, they provide all the information on λ that can be obtained from the eigenvalues of the Casimir operators, namely, they fix the values of $l_1 l_2$ and $l_1 l_2(l_1 + l_2)$. Note that a finite-dimensional irreducible representation of $\mathrm{spl}(2,1)$ is typical[10,11] if and only if $l_1 l_2 \neq 0$.

Remark 1: If C is a Casimir element without a constant term, then the corresponding polynomial function c is divisible by $c_2 = -2l_1 l_2$. This is a special feature of the algebra $\mathrm{spl}(2,1)$.

Remark 2: The algebra $\mathrm{spl}(2,1)$ is well suited to visualize several other of our foregoing investigations. For example, we suggest to derive the relation for the functions c_n which stems from the fact that the matrix A satisfies its own characteristic equation [see Eq. (7.18) of Ref. 2].

The reader will anticipate that the techniques applied above should work for all the Lie superalgebras investigated in this paper. This seems to be the case, and some partial results have already been obtained.[13] We hope to return to these questions in a future publication.

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Anisotropic cosmological model with viscous fluid

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We present an exactly solvable Bianchi type I cosmological model with a viscous fluid. We show that the role of viscosity is more important in the initial epochs of the universe and, in that same period, pressure is more important than fluid density.

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1. INTRODUCTION

The discovery of the cosmic background radiation[1] made it widely believed that cosmological models had to have extremely hot and dense initial states in order to explain this feature. To investigate cosmological solutions in Einstein's theory one usually chooses the energy-momentum tensor of matter as that due to a perfect fluid. All those models lead to an initial singular state. It is interesting to study cosmological models with a more realistic matter source by taking into account dissipative processes due to viscosity. The introduction of viscosity counteracts gravitational collapse; hence one might expect that the initial state of cosmological models could be changed by this dissipative process.

Murphy[2] obtained the solution for the zero spatial curvature Friedmann cosmological model with bulk viscosity and he showed that the initial singularity could be removed, Treciokas and Ellis[3] also found exact solutions but with constant bulk viscosity coefficient, and Nightingale[4] obtained approximate solutions. Belinskii and Khalatnikov analyzed qualitatively the isotropic cosmological models[5] and the anisotropic Bianchi type I cosmological models[6] under the influence of viscosity. They have shown that in the anisotropic models near the initial state the energy density of matter vanishes and later increases, and this feature is interpreted as a creation of matter by the gravitational field near the initial singularity. Caderni and Fabri[7] analyzed the anisotropic cosmological model by numerical integration.

So far no solution is known for viscous fluid in a Bianchi type I universe. In this paper an attempt is made to find exact solutions under the assumption that $\sigma^2/\Theta^2 = D^2$ is a constant.[8] Small values of D^2 will cause shear to be prominent only when the expansion or collapse rate is very very large, i.e., $|\Theta| \to \infty$. For finite $|\Theta|$, σ is not very significant. The relations between the viscosity coefficients and the energy density given in our paper are assumed following Murphy.[2] Under such restrictions we can obtain a first-order differential equation for the expansion. It is very difficult to obtain solutions for viscous fluid with an equation of state. The restrictions mentioned above in obtaining solutions are mainly geometrical and are made to simplify the calculations, but in the absence of any exact solution our solution is a reasonable attempt.

The model obtained, satisfying Hawking's energy conditions,[9] shows that the role of viscosity is more important near the initial epochs of the universe. Contrary to Belinskii and Khalatnikov's result the energy density of matter becomes infinite in the initial state which starts with a finite radius. Further, we obtained that pressure is more important than fluid density in the initial epochs.

2. EINSTEIN'S FIELD EQUATIONS

The homogeneous anisotropic Bianchi type I space-time is given by

$$ds^2 = dt^2 + e^{2\gamma(t)}dx^2 + e^{2\theta(t)}dy^2 + e^{2\psi(t)}dz^2. \tag{2.1}$$

In this space-time we build a cosmological model with a viscous fluid having the energy-momentum tensor[6] given by

$$\begin{aligned} T_{ij} &= (\rho + \bar{p})v_i v_j + \bar{p}g_{ij} - \eta_s \mu_{ij}, \\ \bar{p} &= p - (\eta_b - \tfrac{2}{3}\eta_s)v^a{}_{;a}, \\ v_i v^i &= -1, \\ \mu_{ij} &= v_{i;j} + v_{j;i} + v_i v^a v_{j;a} + v_j v^a v_{i;a}, \end{aligned} \tag{2.2}$$

where ρ is the matter density, p the pressure, v^i the four-velocity, η_b and η_s are the bulk and shear viscosity coefficients. All these quantities in homogeneous models are only time dependent. Choosing a comoving coordinate frame where $v^i = \delta^i_o$, the nonvanishing components of Einsteins's field equations

$$G^j_i = R^j_i - \tfrac{1}{2}\delta^j_i R = -\kappa T^j_i \tag{2.3}$$

with (2.1) and (2.2) are

$$G^0_0 = \frac{9}{2}\left(\frac{\dot{R}}{R}\right)^2 - \tfrac{1}{2}(\dot{\gamma}^2 + \dot{\theta}^2 + \dot{\psi}^2) = \kappa\rho, \tag{2.4}$$

$$\begin{aligned} G^1_1 &= \ddot{\theta} + \ddot{\psi} + \tfrac{3}{2}(\dot{R}/R)(\dot{\theta} + \dot{\psi} - \dot{\gamma}) \\ &\quad + \tfrac{1}{2}(\dot{\gamma}^2 + \dot{\theta}^2 + \dot{\psi}^2) = \kappa(\bar{p} - 2\eta_s\dot{\gamma}), \end{aligned} \tag{2.5}$$

$$\begin{aligned} G^2_2 &= \ddot{\gamma} + \ddot{\psi} + \tfrac{3}{2}(\dot{R}/R)(\dot{\gamma} + \dot{\psi} - \dot{\theta}) \\ &\quad + \tfrac{1}{2}(\dot{\gamma}^2 + \dot{\theta}^2 + \dot{\psi}^2) = -\kappa(\bar{p} - 2\eta_s\dot{\theta}), \end{aligned} \tag{2.6}$$

$$\begin{aligned} G^3_3 &= \ddot{\gamma} + \ddot{\theta} + \frac{3}{2}\left(\frac{\dot{R}}{R}\right)(\dot{\gamma} + \dot{\theta} - \dot{\psi}) \\ &\quad + \tfrac{1}{2}(\dot{\gamma}^2 + \dot{\theta}^2 + \dot{\psi}^2) = -\kappa(\bar{p} - 2\eta_s\dot{\psi}), \end{aligned} \tag{2.7}$$

where the dot represents time differentiation and R stands for

$$R^3 := \exp(\gamma + \theta + \psi).$$

There are four independent equations (2.4)–(2.7) and seven unknown functions, namely γ, θ, ψ, ρ, p, η_b, and η_s; hence we have here the freedom to assume three appropriate relations between these variables to obtain solutions of the system. Following considerations of fluid mechanics[2,10,11] we

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assume

$$\eta_b = \alpha_b \rho, \quad \eta_s = \alpha_s \rho, \tag{2.8}$$

where α_b and α_s are constants. The third relation is the assumption that the ratio between shear and expansion is constant,

$$\sigma^2/\Theta^2 = D^2. \tag{2.9}$$

We consider small values of D^2 in order to have shear only prominent when the expansion or collapse is $|\Theta| \to \infty$. The expansion and shear are given, respectively, by

$$\Theta = v^i_{;i}, \tag{2.10}$$

$$\sigma^2 = \sigma_{ij}\sigma^{ij}, \tag{2.11}$$

$$\sigma_{ij} = v_{(i;j)} + \tfrac{1}{2}(v_{i;a}v^a v_j + v_{j;a}v^a v_i) - \tfrac{1}{3}\Theta(g_{ij} + v_i v_j),$$

which become with metric (2.1)

$$\Theta = 3\dot{R}/R, \tag{2.12}$$

$$\sigma^2 = \dot{\gamma}^2 + \dot{\theta}^2 + \dot{\psi}^2 - \tfrac{1}{3}\Theta^2. \tag{2.13}$$

Now we give the expressions of the motion equation $T_{i;j}^{j} = 0$ and trace $g_{ij}G^{ij}$ of the field equations (2.3) to help us to obtain the solution

$$T_{i;j}^{j} = -\dot{\rho} - (\rho + \bar{p})\Theta + 2\eta_s(\dot{\gamma}^2 + \dot{\theta}^2 + \dot{\psi}^2) = 0, \tag{2.14}$$

$$g_{ij}G^{ij} = 2\dot{\Theta} + \Theta^2 + \dot{\gamma}^2 + \dot{\theta}^2 + \dot{\psi}^2 = -\kappa(-\rho + 3\bar{p} - 2\eta_s\Theta). \tag{2.15}$$

Eliminating $\bar{p}$ of (2.14) and (2.15) and considering (2.9) we obtain

$$-\kappa\dot{\rho} - \tfrac{4}{3}\kappa\rho\Theta + \tfrac{1}{3}[2\dot{\Theta} + (\tfrac{4}{3} + D^2)\Theta^2]\Theta + 2\kappa D^2\eta_s\Theta^2 = 0. \tag{2.16}$$

Now substituting (2.9) into (2.4) we have

$$\kappa\rho = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2, \tag{2.17}$$

which shows that in order to have $\rho > 0$ we need

$$1/a^2 := 2\alpha_s(\tfrac{1}{3} - \tfrac{1}{2}D^2) > 0. \tag{2.18}$$

Introducing (2.17) and (2.8) into (2.16) we finally obtain

$$\dot{\Theta} + (1/a^2)\Theta^3 + \Theta^2 = 0, \tag{2.19}$$

which by integration gives

$$C_1 - ta^2 = \ln R^3 + C_2R^3, \tag{2.20}$$

where C_1 and C_2 are integration constants. By differentiating (2.20) we obtain

$$\Theta = -a^2(1 + C_2R^3)^{-1}. \tag{2.21}$$

Introducing into (2.14) Eqs. (2.8), (2.9), and (2.19) we obtain

$$\kappa\bar{p} = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2(2\alpha_s\Theta + 1) = \kappa\rho(2\alpha_s\Theta + 1), \tag{2.22}$$

so that

$$\kappa p = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2 + (\alpha_b + \tfrac{4}{3}\alpha_s)(\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^3 = \kappa\rho + (\alpha_b + \tfrac{4}{3}\alpha_s)(\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^3. \tag{2.23}$$

3. INTERPRETATION OF THE SOLUTION

When $D^2 = \tfrac{2}{3}$ we see from (2.17) and (2.23) that $\rho = p = 0$; we get vacuum the solution which gives Kasner's metric. Equation (2.18) is derived on the assumption that $D^2 \neq 0$, but the original equation from which it is derived is

$$D^2(\dot{\Theta} + (1/a^2)\Theta^3 + \Theta^2) = 0. \tag{3.1}$$

So for $D^2 = 0$, i.e., for the isotropic case where $\sigma^2 = 0$, Eq. (3.1) is an identity and the solution is obtained from the field equations.[2] If the model is anisotropic, $D^2 \neq 0$, then we have the equation

$$\dot{\Theta} + (1/a^2)\Theta^3 + \Theta^2 = 0 \tag{3.2}$$

which is Eq. (2.19).

Special cases

(A) $a = \infty$, i.e., $\alpha_s(\tfrac{1}{3} - \tfrac{1}{2}D^2) = 0$

This is true when

Case I: $D^2 = \tfrac{2}{3}$, which gives the vacuum Kasner metric.

Case II: $\alpha_s = 0$, for which the shear viscosity has negligible effect and the bulk viscosity is dominant as in Murphy's case. The difference from Murphy's case is that in our case the model is anisotropic.

For Case II $\alpha_s = 0$, we have

$$\dot{\Theta} + \Theta^2 = 0, \tag{3.3}$$

or after integration

$$\Theta = 1/(t - t_0), \tag{3.4}$$

where t_0 is an integration constant. Since $\Theta = 3\dot{R}/R$, Eq. (3.4) results in

$$R^3 \sim (t - t_0) \tag{3.5}$$

for models represented by (3.4) when $t \to t_0$, $\Theta \to \infty$, and $R \to 0$. At this point both ρ and p increase to indefinitely large values. When $t \to \infty$ then $\Theta \to 0$, $R \to \infty$ and we have the universe exploding from a point singularity to a large dimension and the rate of expansion approaches zero asymptotically. For $t < t_0$, Θ is negative representing collapse and for a certain range of Θ the energy conditions[9] are violated. The energy conditions demand

$$\kappa(\rho + \bar{p}) \geqslant 0 \quad \text{and} \quad \kappa(\rho + 3\bar{p}) \geqslant 0. \tag{3.6}$$

When $\Theta < 0$ we write $\Theta = -|\Theta|$ and in order that both the conditions (3.6) are satisfied one must have

$$|\Theta| < 2/3\alpha_s. \tag{3.7}$$

So the magnitude of Θ cannot exceed the value $2/(3\alpha_s)$. For vanishing shear viscosity ($\alpha_s = 0$) it does not create any problem and we have a collapsing as well as expanding model. But for finite α_s we have only an expanding model valid throughout its life.

For $t \to \infty$, $\Theta \to 0$ and we have

$$\kappa\rho = \kappa\bar{p} = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2 = \frac{\tfrac{1}{3} - \tfrac{1}{2}D^2}{(t - t_0)^2} \quad \text{and} \quad \bar{p} \approx p.$$

On the other hand for $t \to t_0$, $\Theta \to \infty$, and

$$\kappa\rho = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2,$$

$$\kappa p = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2 + \alpha_b(\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^3,$$

so that $p \gg \rho$, the fluid pressure is very very large compared to the matter density near the singularity because of the bulk viscosity.

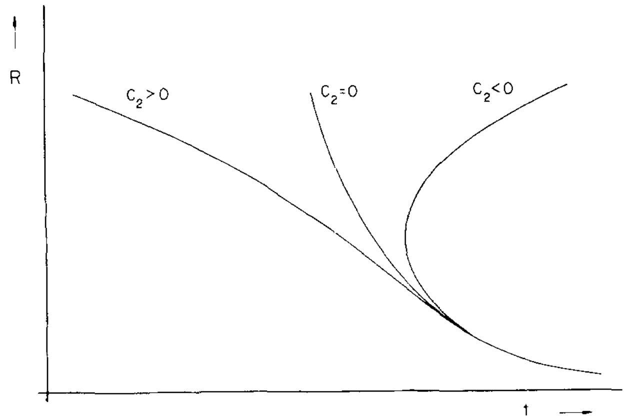

FIG. 1. The $(R-t)$ curve.

(B) $a \neq 0$, *then* $\Theta = -a^2/(1+C_2R^3)$ *and* $\dot{R} = -(a^2R)/(3(1+C_2R^3))$.

Case I: $C_2 > 0$. Since $\Theta = -a^2/(1+C_2R^3)$, $\Theta < 0$ in this case, i.e., it is a collapsing case. When $t \to \infty$, $R \to 0$ and $\Theta \to -a^2$, but $\dot{R}$ approaches zero. When $t \to -\infty$, $R \to \infty$ but $\dot{R} \to 0$. The $(R-t)$ curve is shown in Fig. 1. In order that energy conditions (3.6) are satisfied

$$\Theta < 2/3\alpha_s;$$

that is, one must have $a^2 < 2/(3\alpha_s)$ so that the energy conditions are satisfied at the final stage of collapse $(t \to \infty, R \to 0, \Theta \to -a^2)$. But we have $a^{-2} = 2\alpha_s(\frac{1}{3} - \frac{1}{2}D^2)$, or

$$\alpha_s a^2 = 1/2(\tfrac{1}{3} - \tfrac{1}{2}D^2) > \tfrac{3}{2} \quad \text{or} \quad a^2 > 3/2\alpha_s.$$

Hence we conclude that the energy conditions are not satisfied at least near the final stage of collapse.

Case II: $C_2 = 0$. Then we have from (2.20)

$$\ln R^3 = -a^2t + C_1 \quad \text{or} \quad R = \exp(-\tfrac{1}{3}a^2t + \tfrac{1}{3}C_1),$$

and

$$\Theta = -a^2 \quad \text{or} \quad \dot{R} = -\tfrac{1}{3}a^2R.$$

Then density ρ [(2.17)] and the fluid p [(2.33)] are constants, i.e., independent of time, although R decreases in the course of time. It is also a collapsing case. The $(R-t)$ curve is an exponential curve. Since $\Theta = -a^2$, we have here $|\Theta| = a^2 > 3/(2\alpha_s)$. In order that energy conditions (3.6) are satisifed $|\Theta| < 2/3\alpha_s$. So this collapsing model does not satisfy the Hawking energy conditions.[9]

Case III: $C_2 < 0$. Let us write $C_2 = -|C_2|$. Then from (2.20)

$$C_1 - a^2t = \ln R^3 - |C_2|R^3,$$

$$\Theta = -\frac{a^2}{1-|C_2|R^3},$$

$$\dot{R} = -\frac{a^2}{3}\frac{R}{1-|C_2|R^3}.$$

When $|C_2|R^3 = 1$, i.e., $R^3 = 1/|C_2|$, we have $\Theta \to \infty$, and $\Theta \to 0$ only when $R \to \infty$. $\dot{R} > 0$ for $|C_2|R^3 > 1$ and so once R increases from $R = R_0$, where $R_0^3 = 1/|C_2|$, it will continue to increase till $R \to \infty$. This is an expanding model. During the expansion phase

$$\Theta = \frac{a^2}{|C_2|R^3 - 1} > 0, \quad \dot{R} = \frac{a^2}{3}\frac{R}{|C_2|R^3-1} > 0.$$

As R increases Θ becomes smaller and smaller. When $R \to \infty$, $\Theta \to 0$, $\dot{R} = \frac{1}{3}a^2R/(|C_2|R^3 - 1) \approx a^2/(3|C_2|R^3)$, i.e., $\dot{R} \to 0$. The universe expands from a finite volume and finally tends to infinite dimension and the rate of expansion gradually slows down. Since $\Theta > 0$, in this case energy conditions (3.6) are satisfied throughout the evolution. When $R^3 \to 1/|C_2|$, $\Theta \to \alpha$ and we have singularities of ρ and p. But, from (2.17) and (2.23),

$$\kappa\rho = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2,$$

$$\kappa p = (\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^2 + (\alpha_b + \tfrac{4}{3}\alpha_s)(\tfrac{1}{3} - \tfrac{1}{2}D^2)\Theta^3.$$

So when $\Theta \to \infty$, $p \gg \rho$ for finite viscosity coefficients and the fluid pressure is more important than the fluid density. On the other hand for $t \to \infty$ then $R \to \infty$, $\Theta \to 0$ and we have from (2.20), (2.17), and (2.23),

$$a^2t \approx |C_2|R^3,$$

$$\kappa\rho \approx (\tfrac{1}{3} - \tfrac{1}{2}D^2)/t^2 \to 0,$$

$$\kappa p \approx (\tfrac{1}{3} - \tfrac{1}{2}D^2)/t^2 \to 0.$$

The effects of viscosity appear only in the term of the order of $1/t^3$ and so is negligible.

When $|C_2|R^3 < 1$, $\Theta < 0$ and it is a collapsing case. R decreases continuously without any turning point from $R^3 = 1/|C_2|$ to $R \to 0$, when $\Theta \to -a^2$. At this final stage of collapse the energy conditions are violated as has been shown earlier.

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