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Expectation Value Formalism in Quantum Field Theory. I

PRADIP M. BAKSHI AND KALYANA T. MAHANTHAPPA*†
Lyman Laboratories, Harvard University, Cambridge, Massachusetts
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A formalism has been developed to evaluate the expectation values of projection operators directly. The formalism is applied to the production of particles when the corresponding quantized fields are coupled to external sources and external electromagnetic fields.

I. INTRODUCTION

EXPERIMENTALLY observable quantities are the expectation values of the corresponding projection operators. It has long been asked whether one cannot evaluate the expectation values directly, instead of squaring the corresponding amplitudes. Recently, Schwinger[1] has extended the quantum action principle to achieve this end.

In this and the following papers, a formalism has been developed to evaluate the expectation values directly as applicable to the quantum field theory. Before going into the finer details of the formalism, a few words are in order concerning the extension of the quantum action principle. The usual field theoretic procedure for obtaining the expectation values involves the evaluation of the transformation function[2] $\langle\alpha_1'\sigma_1 \mid \alpha_2'\sigma_2\rangle$ (α_1' and α_2' being the eigenvalues of the physical quantities on the space-like surfaces σ_1 and σ_2), followed by an expansion in terms of complete set of states.

Schwinger's extension of the action principle avoids this laborious procedure by considering the temporal development of the physical system in a closed cycle in time (this being only a mathematical contrivance), in which the development from the initial time to the final time is governed by a dynamics different from the other part of the cycle (the return path). More explicitly, consider the differential characterization of the transformation function in virtue of the quantum action principle:

$$\delta\langle\alpha_1'\sigma_1 \mid \alpha_2'\sigma_2\rangle = i\langle\alpha_1'\sigma_1 \mid \delta W_{12} \mid \alpha_2'\sigma_2\rangle,$$

where

$$W_{12} = \int_{\sigma_2}^{\sigma_1} d^4x L(x),$$

$L(x)$ being the Lagrange function for the physical system. For a closed cycle, we have

$$\begin{aligned}\delta\langle\alpha_2''\sigma_2 \mid \alpha_2'\sigma_2\rangle &= \delta \sum_{\beta'} \langle\alpha_2''\sigma_2 \mid \beta'\sigma_1\rangle\langle\beta'\sigma_1 \mid \alpha_2'\sigma_2\rangle \\ &= \delta[\delta(\alpha_2''\alpha_2')] \\ &= 0.\end{aligned}$$

Instead, let the Lagrange function for the temporal development from σ_2 to σ_1 be L_+ and from σ_1 to σ_2 be L_-. Then:

$$\delta\langle\alpha_2''\sigma_2 \mid \alpha_2'\sigma_2\rangle = i\langle\alpha_2''\sigma_2 \mid \delta(W_{12})_+ - \delta(W_{12})_- \mid \alpha_2'\sigma_2\rangle. \quad (1)$$

The integration of this characterization gives the

* Work done while a Faculty of Arts and Sciences Fellow, Harvard University (1960–1961).

† Present address: Department of Physics, University of California, Los Angeles, California.

[1] J. Schwinger, Lectures delivered at the Institute of Theoretical Physics at Brandeis University, summer of 1960; (unpublished); Proc. Natl. Acad. Sci. U. S. **46**, 1401 (1961); J. Math. Physics **2**, 407 (1961).

[2] J. Schwinger, Phys. Rev. **91**, 713 (1953); **91**, 728 (1953); **92**, 1283 (1953); **93**, 615 (1954); **94**, 1362 (1954).

transformation function by which we can generate the expectation value of the projection operator referring to the physical quantity of interest. Besides this computational aspect of the extension, completeness and the principle of causality come out as the natural consequences of the physical boundary conditions which the field in question should satisfy. Another virtue of this method is that because the expectation value is evaluated directly, the effect of the presence of all the physically possible complete sets of states in the theory is naturally taken into account. Thus, the application of this formalism to the quantum electrodynamical problems does not lead to any infrared divergence.

In the next section, we shall delineate some of the finer points of the formalism by considering the simple case of the production of scalar mesons in the presence of an external source. Here, we evaluate the probability of production of a certain number of mesons when the source is present between the surfaces σ_1 and σ_2 but leaves the meson field in isolation on the surfaces. The problem is solved in three stages: (i) construction of proper projection operators; (ii) integration of the differential characterization of $\langle \sigma_2 \mid \sigma_2 \rangle$; and (iii) generation of the expectation values of the projection operators. The last stage will not be carried out in the next section, as this is the same for the production of photons which will be dealt with in detail in Sec. III. In Secs. IV and V we shall treat the problems of pair production of charged mesons and fermions in the presence of an external electromagnetic field. In the following paper,[3] a formalism for coupled fields will be given.

II. PRODUCTION OF NEUTRAL SCALAR MESONS IN THE PRESENCE OF AN EXTERNAL SOURCE

The Lagrange function for a scalar meson field ϕ in the presence of an external source ζ is

$$L(x) = -\pi_\mu \, \partial_\mu \phi + \tfrac{1}{2}(\pi_\mu^2 + \mu^2 \phi^2) + \phi \zeta .$$

By the application of the action principle, we have for the field equations (with $\mu = 1, 2, 3, 4$)

$$\begin{aligned} \partial_\mu \phi &= \pi_\mu , \\ -\partial_\mu \pi_\mu &= -\mu^2 \phi + \zeta , \end{aligned} \tag{2a}$$

and the generators

$$\begin{aligned} G_\phi &= -\int d\sigma_\mu \pi_\mu \, \delta\phi , \\ G_\pi &= \int d\sigma_\mu \, \delta\pi_\mu \phi . \end{aligned} \tag{2b}$$

[3] P. M. Bakshi and K. T. Mahanthappa, following paper, J. Math. Phys. 4, 12 (1963).

In the absence of the source ζ, the field equations are

$$\begin{aligned} \partial_0 \phi &= -\pi_0 \\ \partial_0 \pi_0 &= \mathcal{E}^2 \phi , \end{aligned} \tag{3}$$

where

$$\mathcal{E} = \{(-i \, \partial_k)^2 + \mu^2\}^{1/2} .$$

$\mathcal{E}$ is a Hermitian coordinate operator. Let

$$\phi = \phi^{(+)} + \phi^{(-)} ,$$

and

$$i \, \partial_0 \phi^{(\pm)} = K_\pm \phi^{(\pm)} .$$

Using Eq. (3), we have

$$\begin{aligned} \pi_0 &= iK_+ \phi^{(+)} + iK_- \phi^{(-)} \\ &= \pi^{(+)} + \pi^{(-)} , \end{aligned}$$

and

$$K_\pm = \mathcal{E}^2 ,$$

giving

$$K_+ = \mathcal{E} , \qquad K_- = -\mathcal{E} .$$

Hence, we have

$$i \, \partial_0 \phi^{(\pm)} = \pm \mathcal{E} \phi^{(\pm)} ,$$

and

$$\phi^{(\pm)\dagger} = \phi^{\dagger(\pm)} . \tag{4}$$

Thus, $\phi^{(\pm)}$ represent the positive and negative frequency parts of the field ϕ. The corresponding projection operators are given by

$$P^{(\pm)} = \tfrac{1}{2}(1 \pm \mathcal{E}/E) , \tag{5}$$

where

$$E = (\mathcal{E}^2)^{1/2} .$$

Using (2b) and (4), the generators $G_\pm$ can be written as

$$\begin{aligned} G_+ &= 2i \, \delta\phi^{(+)} \mathcal{E} \phi^{(-)} , \\ G_- &= -2i \phi^{(+)} \mathcal{E} \, \delta\phi^{(-)} , \end{aligned}$$

which imply the following commutation relations on the surface σ:

$$\begin{aligned} &[\phi^{(+)}(x), \phi^{(+)}(x')] = 0 = [\phi^{(-)}(x), \phi^{(-)}(x')] , \\ &[\phi^{(+)}(x), \phi^{(-)}(x')] = (1/2\mathcal{E}) \, \delta_0(x - x') . \end{aligned}$$

Now the transformation function $\langle \phi^{(-)\prime}\sigma_1 \mid \phi^{(+)\prime}\sigma_2 \rangle$ is given by

$$\langle \phi^{(-)\prime}\sigma_1 \mid \phi^{(+)\prime}\sigma_2 \rangle = \exp\Big[\sum_p e^{ipX} \phi_p^{(-)\prime} \phi_p^{(+)\prime}\Big] , \tag{6}$$

where X is the translation which brings the point x_2 on σ_2 into the point x_1 on σ_1, and

$$\phi_p^{(+)\prime} = 2\int_{\sigma_2} d\sigma\phi^{(+)\prime}(x)\,\mathcal{E}\phi_p^*(x)e^{ipx_2},$$
$$\phi_p^{(-)\prime} = 2\int_{\sigma_1} d\sigma\phi^{(-)\prime}(x)\,\mathcal{E}\phi_p(x)e^{-ipx_1}, \tag{7a}$$

where

$$\phi_p^*(x) = \left(\frac{d^3p}{(2\pi)^3}\frac{1}{2\mathcal{E}_p}\right)^{1/2} e^{-ipx},$$
$$\phi_p(x) = \left(\frac{d^3p}{(2\pi)^3}\frac{1}{2\mathcal{E}_p}\right)^{1/2} e^{ipx}, \tag{7b}$$

and

$$\mathcal{E}_p = (\mathbf{p}^2 + \mu^2)^{1/2}.$$

Now one can write

$$\phi'(x) = \phi^{(+)\prime}(x) + \phi^{(-)\prime}(x)$$
$$= \sum_p \phi_p(x)\phi_p^{(+)\prime}e^{-ipx_2} + \sum_p \phi_p^*(x)\phi_p^{(-)\prime}e^{ipx_1}.$$

From (6), one easily gets

$$\langle\phi^{(-)\prime} \mid n\rangle = \prod_p \frac{(\phi_p^{(-)\prime})^{n_p}}{(n_p!)^{1/2}};$$
$$\langle n \mid \phi^{(+)\prime}\rangle = \prod_p \frac{(\phi_p^{(+)\prime})^{n_p}}{(n_p)^{1/2}}, \tag{8}$$

where n_p being the occupation number in the pth mode and $n = \sum n_p$. The projection operator for n particle states $P_n = |n\rangle\langle n|$ can be constructed in terms of $\phi_p^{(*)}$ by considering

$$\langle\phi^{(-)\prime}|P_n|\phi^{(+)\prime}\rangle = \prod_p \frac{(\phi_p^{(-)\prime})^{n_p}}{(n_p!)^{1/2}}\frac{(\phi_p^{(+)\prime})^{n_p}}{(n_p!)^{1/2}}$$
$$= \prod_p \frac{(\phi_p^{(-)\prime})^{n_p}}{(n_p!)^{1/2}}\langle\phi^{(-)\prime} \mid \phi^{(+)\prime}\rangle$$
$$\times \exp\left[-\phi_p^{(-)\prime}\phi_p^{(+)\prime}\right]\frac{(\phi_p^{(+)\prime})^{n_p}}{(n_p!)^{1/2}}$$
$$= \left\langle\phi^{(-)\prime}\left|\prod_p \frac{(\phi_p^{(-)})^{n_p}}{(n_p!)^{1/2}}\right.\right.$$
$$\left.\left.\times \exp\left[-\phi_p^{(-)};\phi_p^{(+)}\right]\frac{(\phi_p^{(+)})^{n_p}}{(n_p!)^{1/2}}\right|\phi^{(+)\prime}\right\rangle,$$

so that

$$P_n = \prod_p \frac{(\phi_p^{(-)})^{n_p}}{(n_p!)^{1/2}} \exp\left[-\phi_p^{(-)};\phi_p^{(+)}\right]\frac{(\phi_p^{(+)})^{n_p}}{(n_p!)^{1/2}}$$
$$= \prod_p P_{n_p}, \tag{9}$$

where ; refers to the fact that on expansion of the exponential all the $\phi_p^{(-)}$'s are to the left and the $\phi_p^{(+)}$'s are to the right. The projection operator for the state referring to n particles with no distinction of modes is given by

$$P_n = \sum_{n_p}\prod_p P_{n_p}, \tag{10a}$$

with

$$\sum_p n_p = n.$$

A convenient generating function for this set of projection operators is given by

$$Q(\lambda) = \sum_{n=0}^{\infty}\lambda^n \sum_{n_p}\prod_p P_{n_p}, \quad (\text{with} \quad \sum_p n_p = n),$$
$$= \prod_p \exp\left[(\lambda - 1)\phi_p^{(-)};\phi_p^{(+)}\right]$$
$$= \exp\left[(\lambda - 1)\sum_p \phi_p^{(-)};\phi_p^{(+)}\right]. \tag{10b}$$

Now we shall construct the transformation function $\langle\sigma_2 \mid \sigma_2\rangle_\theta^*$ with the source ζ_+ from σ_2 to σ_1 and ζ_- from σ_1 to σ_2, θ referring to the fact that the given initial state is a thermal mixture. From (2a) we have for

$$[(-i\,\partial_\mu)^2 + \mu^2]\langle\phi\rangle = \zeta, \tag{11a}$$

and the corresponding equation for Green's function is

$$[(-i\,\partial_\mu)^2 + \mu^2]G(xx') = \delta(x - x'). \tag{11b}$$

The Green's functions in which we would be interested are the retarded, the advanced, the causal and the anticausal Green's functions, indicated, respectively, by G^r, G^a, $G^{(+)}$ and $G^{(-)}$. They are given, in terms of the mode functions (7b), by

$$G^r(xx') = i(S^{(+)} - S^{(-)})(xx')\eta_+(xx'),$$
$$G^a(xx') = -i(S^{(+)} - S^{(-)})(xx')\eta_-(xx'),$$
$$G^+(xx') = iS^{(+)}(xx')\eta_+(xx') + iS^{(-)}(xx')\eta_-(xx'), \tag{12a}$$
$$G^-(xx') = -iS^{(+)}(xx')\eta_-(xx') - iS^{(-)}(xx')\eta_+(xx'),$$

where

$$S^{(+)}(xx') = \sum_p \phi_p(x)\phi_p^*(x'),$$
$$S^{(-)}(xx') = \sum_p \phi_p^*(x)\phi_p(x'),$$

and $\eta_+(xx')$ and $\eta_-(xx')$ are Heaviside step functions. In order to get the required transformation function, we have to solve (11a), subject to the following boundary conditions:

(i) For $t \geq t_1$, $\zeta_+ = \zeta_-$ and hence,

$$\langle(\phi_-^{(*)} - \phi_+^{(*)})(t)\rangle = 0, \quad \text{for} \quad t \geq t_1; \tag{13a}$$

(ii) For $t < t_2$, the expectation values of field operators are zero:

$$\langle\phi_-(t)\rangle = 0 = \langle\phi_+(t)\rangle, \quad \text{for} \quad t < t_2; \tag{13b}$$

(iii) The frequency conditions are obtained as follows. There exists an operator U such that

$$\langle\sigma_2 \mid \sigma_2\rangle^* = \langle\sigma_2 \mid U \mid \sigma_2\rangle.$$

Hence, with the thermal mixture for the initial state[4]

$$\langle\sigma_2 \mid \phi_-^{(*)} \mid \sigma_2\rangle = \frac{\mathrm{Tr}\,[\exp(-\beta H_0)\phi^{(*)}U]}{\mathrm{Tr}\exp(-\beta H_0)},$$

$$\langle\sigma_2 \mid \phi_+^{(*)} \mid \sigma_2\rangle = \frac{\mathrm{Tr}\,[\exp(-\beta H_0)U\phi^{(*)}]}{\mathrm{Tr}\exp(-\beta H_0)},$$

where H_0 is the Hamiltonian of the system and $\beta = i\tau = 1/\theta$ is a measure of temperature when β is real and positive; the trace is the grand canonical average. We have for the evolution of the field operators:

$$\exp[i(t-t_2)H_0]\phi^{(*)}(t_2)\exp[-i(t-t_2)H_0] = \phi^{(*)}(t) = \exp[\pm i\varepsilon(t-t_2)]\phi^{(*)}(t_2).$$

With $(t - t_2) \to i\beta$, we have

$$\exp(-\beta H_0)\phi^{(*)}(t_2)\exp(\beta H_0) = \exp[\mp i\varepsilon(t-t_2)]\phi^{(*)}(t_2),$$

or

$$\exp(-\beta H_0)\phi^{(*)}(t_2)U = \exp[\mp i\varepsilon(t-t_2)]\phi^{(*)}(t_2)\exp(-\beta H_0)U.$$

Taking traces on both sides, we have

$$\langle\phi_-^{(*)}(t_2)\rangle = \langle\exp(\pm\beta\varepsilon)\phi_+^{(*)}(t_2)\rangle,$$

which can be written as

$$\langle(\phi_- + \phi_+)(t_2)\rangle = \epsilon(\lambda)\langle\coth\beta\varepsilon(\phi_- - \phi_+)(t_2)\rangle, \tag{13c}$$

where $\epsilon(\lambda) = \lambda/|\lambda|$ and $\lambda = \pm 1$ for positive and negative frequency parts.

The most general solution of Eq. (11a) is given by

$$\langle\phi(x)\rangle = \int_{\sigma_2}^{\sigma_1} d^4x' G(x, x')\zeta(x') - \int_{\sigma_2} d\sigma_2 G(x, x_2)\cdot\frac{\partial\phi(x_2)}{\partial x_{20}}, \tag{14}$$

where

$$G(xx_2)\cdot\frac{\partial\phi(x_2)}{\partial x_{20}} = G(xx_2)\frac{\partial\phi(x_2)}{\partial x_{20}} - \frac{\partial G(xx_2)}{\partial x_{20}}\phi(x_2).$$

From the continuity condition (13a), we have

$$(\phi_- - \phi_+)(x) = \int_{\sigma_2}^{\sigma_1} d^4x' G^a(xx')(\zeta_- - \zeta_+)(x'). \tag{15a}$$

From (13b), we have

$$\phi_*(x) = \int_{\sigma_2}^{\sigma_1} d^4x' G^r(xx')\zeta_*(x') - \int_{\sigma_2} d\sigma_2 G^r(xx_2)\cdot\frac{\partial\phi_*(x_2)}{\partial x_{20}}. \tag{15b}$$

This, combined with (13c), (15a), and (15b), gives

$$(\phi_- - \phi_+)(x) = \int_{\sigma_2}^{\sigma_1} d^4x' G^r(xx')(\zeta_- + \zeta_+)(x') + \int_{\sigma_2}^{\sigma_1} d^4x' W_\theta(xx')(\zeta_- - \zeta_+)(x'), \tag{15c}$$

where

$$W_\theta(xx') = \int_{\sigma_2} d\sigma_2 G^r(xx_2)\cdot\frac{\partial}{\partial x_{20}} \times [(P^{(+)} - P^{(-)})\coth\tfrac{1}{2}\beta\varepsilon G^a(x_2x')].$$

The differential characterization of the transformation function $\langle\sigma_2 \mid \sigma_2\rangle^*$, by virtue of the action principle, is

$$\delta\langle\sigma_2 \mid \sigma_2\rangle_\theta^* = i\left\langle\left|\int_{\sigma_2}^{\sigma_1}(\delta\zeta_+\phi_+ - \delta\zeta_-\phi_-)\right|\right\rangle_\theta^*. \tag{16a}$$

Then we have

$$\pm(1/i)[\delta/\delta\zeta_*(x)]\langle 1\rangle_\theta^* = \langle|\phi_*(x)|\rangle_\theta^*. \tag{16b}$$

Equation (16a) can be written as

$$\delta\langle|\rangle_\theta^* = -\frac{i}{2}\left\langle\left|\int_{\sigma_2}^{\sigma_1}\delta(\zeta_- + \zeta_+)(x)(\phi_- - \phi_+)(x) + \delta(\zeta_- - \zeta_+)(x)(\phi_- + \phi_+)(x)\right|\right\rangle_\theta^*. \tag{16c}$$

Making use of Eqs. (15), we have

$$\begin{aligned}\delta\langle|\rangle_\theta^* = -\frac{i}{2}\Big\langle\Big|\int_{\sigma_2}^{\sigma_1}&\delta(\zeta_- - \zeta_+)(x)G^r(xx')(\zeta_- + \zeta_+)(x') \\ &+ (\zeta_- - \zeta_+)(x')G^a(xx')\,\delta(\zeta_- + \zeta_+)(x) \\ &+ \delta(\zeta_- - \zeta_+)(x)W_\theta(xx')(\zeta_- - \zeta_+)(x')\Big|\Big\rangle_\theta^* \\ = -\frac{i}{2}\Big\langle\Big|\delta\int_{\sigma_2}^{\sigma_1}&[(\zeta_- - \zeta_+)(x(G^r(xx')(\zeta_- + \zeta_+)(x') \\ &+ \tfrac{1}{2}(\zeta_- - \zeta_+)(x)W_\theta(xx')(\zeta_- - \zeta_+)(x')]\Big|\Big\rangle_\theta^*.\end{aligned}$$

Performing the functional integration, we have

$$\langle\sigma_2 \mid \sigma_2\rangle_\theta^* = \exp[(i/2)\zeta G_\theta\zeta^\dagger], \tag{17}$$

where

[4] P. C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959).

$$\zeta = \widetilde{\zeta_+ \quad \zeta_-}; \qquad \zeta^\dagger = \begin{pmatrix}\zeta_+ \\ \zeta_-\end{pmatrix},$$

and

$$G_\theta = \begin{pmatrix}G_{++} & G_{+-} \\ G_{-+} & G_{--}\end{pmatrix},$$

where

$$\left.\begin{aligned}
G_{++} &= (G^r - \tfrac{1}{2}W_\theta) = (G^a - \tfrac{1}{2}W_\theta) \\
&= \tfrac{1}{2}(G^r + G^a - W_\theta), \\
G_{+-} &= (G^r + \tfrac{1}{2}W_\theta) = -(G^a - \tfrac{1}{2}W_\theta) \\
&= \tfrac{1}{2}(G^r - G^a + W_\theta), \\
G_{-+} &= -(G^r - \tfrac{1}{2}W_\theta) = (G^a + \tfrac{1}{2}W_\theta) \\
&= \tfrac{1}{2}(G^a - G^r + W_\theta), \\
G_{--} &= -(G^r + \tfrac{1}{2}W_\theta) = -(G^a + \tfrac{1}{2}W_\theta) \\
&= -\tfrac{1}{2}(G^r + G^a + W_\theta).
\end{aligned}\right\} \tag{18}$$

In Eqs. (18), the equalities between various combinations of G^r, G^a and W_θ must be understood as being true under the integral in the exponential of Eq. (17). By virtue of Eq. (16b), we have

$$\begin{aligned}
-i\frac{\delta}{\delta\zeta_\pm(x)}\frac{\delta}{\delta\zeta_\pm(x')}\langle|\rangle_\theta^{\pm}\,|_{\zeta=0} \\
= G_{\pm\pm} = i\langle(\phi(x)\phi(x'))_\pm\rangle_\theta, \\
-i\frac{\delta}{\delta\zeta_\pm(x)}\frac{\delta}{\delta\zeta_\mp(x')}\langle|\rangle_\theta^{\pm}\,|_{\zeta=0} \\
= G_{\pm\mp} = -i\begin{cases}\langle(\phi(x')\phi(x))\rangle_\theta \\ \langle(\phi(x)\phi(x'))\rangle_\theta.\end{cases}
\end{aligned} \tag{19}$$

Here, $(\,)_+$ and $(\,)_-$ mean positive and negative time ordering. Now, if $\zeta_+ = \zeta_-$, we have

$$\langle\sigma_2 \mid \sigma_2\rangle_\theta = 1, \tag{20}$$

which requires that the sum of the elements of G_0,

$$G_{++} + G_{+-} + G_{-+} + G_{--} = 0 \tag{21}$$

This is the statement of completeness.

It is easily seen that the transformation function can be expressed as

$$\langle\sigma_2 \mid \sigma_2\rangle_\theta^{\pm} = \left\langle\left|\left(\exp\left(-i\int\zeta_-\phi_-\right)\right)_-\left(\exp\left(i\int\zeta_+\phi_+\right)\right)_+\right|\right\rangle_\theta.$$

Now

$$\begin{aligned}
&\frac{1}{i}\frac{\delta}{\delta\zeta_+(x)}\left(\exp\left(i\int_{\sigma_-\infty}^{\sigma+\infty}\zeta_+\phi_+\right)\right)_+ \\
&= \left[\exp\left(i\int_{\sigma_x}^{\sigma\infty}\zeta_+\phi_+\right)\right]_+\phi_+(x)\left[\exp\left(i\int_{\sigma-\infty}^{\sigma_x}\zeta_+\phi_+\right)\right]_+.
\end{aligned}$$

Hence,

$$\begin{aligned}
\langle\phi(x)\rangle_\theta^\zeta &= \frac{1}{i}\frac{\delta}{\delta\zeta_+(x)}\langle\sigma_2 \mid \sigma_2\rangle_\theta^{\pm}\,|_{\zeta_+=\zeta=\zeta_-} \\
&= \left\langle\left[\exp\left(-i\int_{\sigma-\infty}^{\sigma_x}\zeta\phi\right)\right]_-\phi(x)\left[\exp\left(i\int_{\sigma-\infty}^{\sigma_x}\zeta\phi\right)\right]_+\right\rangle_\theta
\end{aligned}$$

and

$$\frac{\delta}{\delta\zeta(x')}\frac{\delta}{\delta\zeta_+(x)}\langle|\rangle_\theta^{\pm}\,|_{\zeta_+=\zeta=\zeta_-} = 0, \quad \text{for} \quad t' > t, \tag{22}$$

thus indicating that the expectation value of $\phi(x)$ is dependent on the history of the system up to the time t, which is an expression of causality.

III. PRODUCTION OF PHOTONS IN THE PRESENCE OF AN EXTERNAL CURRENT

The Lagrange function for the electromagnetic field with potential A_μ in the presence of an external current K_μ, is given by

$$L(x) = \tfrac{1}{4}F_{\mu\nu}^2 - \tfrac{1}{4}\{F_{\mu\nu}, \partial_\mu A_\nu - \partial_\nu A_\mu\} + K_\mu A_\mu.$$

The application of the action principle yields two sets of equations with no time derivatives. Proceeding in the usual fashion,[2] to eliminate the longitudinal part of the field, we get for transverse field, without the source,

$$\begin{aligned}
-\partial_0 A_k &= F_{0k}, \\
\partial_0 F_{0k} &= \omega^2 A_k,
\end{aligned}$$

where

$$\omega = [(-i\,\partial_l)^2]^{1/2}.$$

In the coordinate representation, ω can be written as

$$\langle x \mid\omega\mid x'\rangle = \int\frac{d^3k}{(2\pi)^3}\,|\mathbf{k}|\,e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')},$$

which is symmetrical and positive definite. As in the case of neutral scalar mesons, we have

$$\partial_0 A^{(\pm)}(x) = \mp i\omega A^{(\pm)}(x),$$

where

$$A^{(\pm)}(x) = \tfrac{1}{2}[A_k \mp (i/\omega)F_{0k}].$$

The corresponding projection operators are

$$P^{(\pm)} = \tfrac{1}{2}[1 \pm \omega/E],$$

with

$$E = (\omega^2)^{1/2}.$$

The corresponding generators are

$$G_\pm = \pm 2i\int d\sigma A^{(\mp)}\omega\,\delta A^{(\pm)},$$

which imply the commutation relations on σ:

$$[A_k^{(+)}(x), A_l^{(+)}(x')] = 0 = [A_k^{(-)}(x), A_l^{(-)}(x')],$$
$$[A_k^{(+)}(x), A_l^{(-)}(x')] = [(1/2\omega)\ \delta_{\sigma kl}(x - x')]^T.$$

It is easily seen that the transformation function $\langle A^{(-)'}\sigma_1 \mid A^{(+)'}\sigma_2\rangle$ is given by[2]

$$\langle A^{(-)'}\sigma_1 \mid A^{(+)'}\sigma_2\rangle = \exp\Big[\sum_{\rho k} e^{ikx} a_{\rho k}^{(-)'} a_{\rho k}^{(+)'}\Big], \tag{23}$$

where

$$a_{\rho k}^{(-)'} = 2\int_{\sigma_1} d\sigma A_\mu^{(-)'}(x)\omega A_{\rho k\mu}(x)e^{-ikx_1},$$

$$a_{\rho k}^{(+)'} = 2\int_{\sigma_2} d\sigma A_\mu^{(+)'}(x)\omega \bar{A}_{\rho k\mu}(x)e^{ikx_2},$$

where

$$A_{\rho k\mu}(x) = \left(\frac{d^3k}{(2\pi)^3}\frac{1}{2k_0}\right)^{1/2} e_\mu(\rho k)e^{ikx},$$

$$\bar{A}_{\rho k\mu}(x) = \left(\frac{d^3k}{(2\pi)^3}\frac{1}{2k_0}\right)^{1/2} e_\mu(\rho k)e^{-ikx},$$

and $k_0 = |\mathbf{k}|$. $e_\mu(\rho k)$ is a pure space vector for $\rho = 1, 2, 3$ and for $\rho = 4$, only the time component exists; first two vectors are orthogonal to $\mathbf{k}$ and the third, parallel. If n_μ is the time-like vector being normal to surface σ_1 and σ_2, we have

$$\rho = 1, 2: \quad n_\mu e_\mu(\rho k) = k_\mu e_\mu(\rho k) = 0,$$
$$e_\mu(3k) = n_\mu + k_\mu/n_\nu k_\nu, \quad n_\mu e_\mu(3k) = 0,$$
$$e_\mu(4k) = in_\mu.$$

Now, as before, one can write

$$A'(x) = \sum_{\rho k} A_{\rho k}(x) a_{\rho k}^{(+)'} e^{-ikx_2} + \sum_{\rho k} \bar{A}_{\rho k}(x) a_{\rho k}^{(-)'} e^{ikx_1}.$$

From (23), we have

$$\langle A^{(-)'} \mid n\rangle = \prod_{\rho k} \frac{(a_{\rho k}^{(-)'})^{n_{\rho k}}}{(n_{\rho k}!)^{1/2}};$$

$$\langle n \mid A^{(+)'}\rangle = \prod_{\rho k} \frac{(a_{\rho k}^{(+)'})^{n_{\rho k}}}{(n_{\rho k}!)^{1/2}},$$

giving for the projection operator

$$P_n = |n\rangle\langle n| = \prod_{\rho k} \frac{(a_{\rho k}^{(-)})^{n_{\rho k}}}{(n_{\rho k}!)^{1/2}} \times \exp[-a_{\rho k}^{(-)}; a_{\rho k}^{(+)}] \frac{(a_{\rho k}^{(+)})^{n_{\rho k}}}{(n_{\rho k}!)^{1/2}}. \tag{24a}$$

We shall introduce a generating function $Q(\lambda)$ for P_n:

$$Q(\lambda) = \sum_{n=0}^{\infty} \sum_{n_{\rho k}} \lambda^n P_n, \quad (\text{with } n = \sum_{\rho k} n_{\rho k}) \tag{24b}$$
$$= \exp[(\lambda - 1)\sum_{\rho k} a_{\rho k}^{(-)}; a_{\rho k}^{(+)}].$$

The field equation for $\langle A_\mu(x)\rangle$ is

$$-\partial_\nu^2\langle A_\mu(x)\rangle = K_\mu(x). \tag{25}$$

The corresponding equation for Green's function is

$$-\partial_\nu^2 D(xx') = \delta(x - x').$$

The relevant Green's functions are given by

$$\begin{aligned} D^r(xx') &= i(\mathrm{S}^{(+)} - \mathrm{S}^{(-)})(xx')\eta_+(xx'), \\ D^a(xx') &= -i(\mathrm{S}^{(+)} - \mathrm{S}^{(-)})(xx')\eta_-(xx'), \\ D^{(+)}(xx') &= i\mathrm{S}^{(+)}(xx')\eta_+(xx') + i\mathrm{S}^{(-)}(xx')\eta_-(xx'), \\ D^{(-)}(xx') &= -i\mathrm{S}^{(+)}(xx')\eta_-(xx') - i\mathrm{S}^{(-)}(xx')\eta_+(xx'), \end{aligned} \tag{26}$$

where

$$\mathrm{S}^{(+)}(xx') = \sum_{\rho k} A_{\rho k}(x)\bar{A}_{\rho k}(x'),$$
$$\mathrm{S}^{(-)}(xx') = \sum_{\rho k} \bar{A}_{\rho k}(x)A_{\rho k}(x).$$

The solutions of (25) must satisfy the boundary conditions similar to Eqs. (13). As before, we get

$$(A_- - A_+)(x) = \int_{\sigma_2}^{\sigma_1} d^4x'\ D^a(xx')(K_- - K_+)(x'),$$

and

$$(A_- + A_+)(x) = \int_{\sigma_2}^{\sigma_1} d^4x'\ D^r(xx')(K_- + K_+)(x') + \int_{\sigma_2}^{\sigma_1} d^4x' W_\theta(xx')(K_- - K_+)(x'), \tag{27}$$

where

$$W_\theta(xx') = -\int_{\sigma_2} d\sigma\ D^r(xx_2)\cdot\frac{\partial}{\partial x_{20}} \times [(P^{(+)} - P^{(-)})\coth \tfrac{1}{2}\beta\omega\ D^a(x_2x')].$$

Making use of the above equations in the differential characterization of the transformation function

$$\delta\langle\sigma_2 \mid \sigma_2\rangle_\theta^{\sigma_1} = i\left\langle\left|\int_{\sigma_2}^{\sigma_1} (\delta K_+ A_+ - \delta K_- A_-)\right|\right\rangle, \tag{28}$$

we get for the transformation function

$$\langle\sigma_2 \mid \sigma_2\rangle_\theta^{\sigma_1} = \exp[(i/2)K\ D_\theta K^\dagger] \tag{29}$$

where

$$K = \overbrace{K_+\ \ K_-}; \qquad K^\dagger = \begin{pmatrix} K_+ \\ K_- \end{pmatrix}$$

$$D_\theta = \begin{pmatrix} D_{++} & D_{+-} \\ D_{-+} & D_{--} \end{pmatrix}$$

with

$$D_{\pm\pm} = \pm(D^r \mp \tfrac{1}{2}W_\theta),$$
$$D_{\pm\mp} = \pm(D^r \pm \tfrac{1}{2}W_\theta).$$

Equations similar to (18) and (19) can be written down. Relations similar to (20), (21), and (22) hold in this case also.

Before evaluating the expectation value of $Q(\lambda)$, we shall make a transformation. Instead of considering the source term $K_\mu A_\mu$ in the Lagrange function, we shall introduce $J^* A^{(+)} + J A^{(-)}$ where $\mathrm{Re}\,(J^* + J) = K$, giving back the original source when the imaginary parts of J and J^* vanish. This transformation leads to

$$\langle \sigma_2 \mid \sigma_2 \rangle_\theta^{J^*} = \exp\,[iJ^*\,\mathfrak{D}_\theta J], \tag{30}$$

where

$$J^* = \overbrace{J_+^*\;\; J_-^*}; \qquad J = \begin{pmatrix} J_+ \\ J_- \end{pmatrix}$$

and

$$\mathfrak{D}_\theta = i \sum_{\rho k} A_{\rho k}(x) \bar{A}_{\rho k}(x') \times \left[\begin{pmatrix} \eta_+(xx') & 0 \\ -1 & \eta_-(xx') \end{pmatrix} + \bar{n}_{\rho k} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \right],$$

where

$$\bar{n}_{\rho k} = [\exp\,(\beta\omega_{\rho k}) - 1]^{-1}$$

For a vacuum $\beta \to \infty$ and $\bar{n}_{\rho k} = 0$. We shall use this transformation function to evaluate the expectation value of $Q(\lambda)$ of Eq. (24b) when the initial state is a vacuum.

$$\langle Q(\lambda) \rangle = \langle \exp\,[(\lambda - 1) \sum_{\rho k} a_{\rho k}^{(-)}; a_{\rho k}^{(+)}] \rangle$$

$$= \prod_{\rho k} \exp\left[-(\lambda - 1) \frac{\partial}{\partial \mu_{\rho k}} \frac{\partial}{\partial \mu_{\rho k}^*} \right] \times \left\langle \exp\left[i \int (\mu^* A^{(+)} + \mu A^{(-)}) \right]_+ \right\rangle \Big|_{\mu^* = 0 = \mu}, \tag{31}$$

where

$$\mu^*(x) = \sum_{\rho k} \bar{A}_{\rho k}(x) \mu_{\rho k}^*,$$

$$\mu(x) = \sum_{\rho k} A_{\rho k}(x) \mu_{\rho k}.$$

The time ordering in (31) refers to the fact that $\mu_{\rho k}$ should appear later than $\mu_{\rho k}^*$ in the limit as we reach the space-like surface σ_1 at which we are evaluating $Q(\lambda)$. In order to generate the expectation value on the right-hand side of Eq. (31), we let

$$J_+^*(x) \to J_+^*(x) + \mu^*(x)\; \delta(t - t_1 + 0),$$

$$J_-(x) \to J_-(x) + \mu(x)\; \delta(t - t_1),$$

which means we are supplementing J_+^* and J_- with impulsive sources. Then we have

$$\langle Q(\lambda) \rangle = \prod_{\rho k} \exp\,[(1 - \lambda)\, \partial_{\rho k}\, \partial_{\rho k}^*] \times \exp\, i(J^*\,\mathfrak{D} J + \mu^*\,\mathfrak{D}_{++} J_+ + J_-^*\,\mathfrak{D}_{--}\mu)\,|_{\mu=0=\mu^*,\,\mathrm{Im}J=0,\,K_+=K=K_-}$$

$$= \exp\,(iJ^*\,\mathfrak{D}J) \times \exp\,[(\lambda - 1) K_+ S K_-]\,|_{K_+=K=K_-}, \tag{32a}$$

where

$$S(xx') = \mathfrak{s}^+(xx') = \sum_{\rho k} A_{\rho k}(x) \bar{A}_{\rho k}(x').$$

$$\langle Q(\lambda) \rangle = \exp\,[(\lambda - 1) KSK] = \prod_k \exp\,[(\lambda - 1)\,|K_k|^2, \tag{32b}$$

where

$$|K_k|^2 = \frac{d^3k}{(2\pi)^3} \frac{1}{2k_0} \left| \int d^4x e^{-ikx} K(x) \right|^2.$$

Here the summation over polarization has been carried out. The probability of n-photon production with the initial vacuum state, $p(n, 0)$, is given by[2,5,6]

$$p(n, 0) = \prod_k \frac{|K_k|^2}{n!} \exp\,[-|K_k|^2]. \tag{33}$$

If we had evaluated $\langle Q(\lambda) \rangle$ for a thermal mixture of initial state, we would get

$$\langle Q(\lambda) \rangle_\theta = \prod_{\rho k} \frac{1}{1 + \bar{n}_{\rho k}(1 - \lambda)} \times \exp\left[(\lambda - 1) \frac{|K_{\rho k}|^2}{1 + \bar{n}_{\rho k}(1 - \lambda)} \right], \tag{34a}$$

where

$$K_{\rho k} = \left(\frac{d^3k}{(2\pi)^3} \frac{1}{2k_0} \right)^{1/2} \int d^4x e_\mu(\rho k) e^{-ikx} K_\mu(x).$$

The extraction of the coefficient of λ^n from (34a) would involve the Laguerre polynomials and the expression, which was first obtained by Schwinger,[2] is

$$p(n, n') = \prod_{\rho k} \frac{n_<!}{n_>!} (|K_{\rho k}|^2)^{n_> - n_<} (L_{n_<}^{n_> - n_<} |K_{\rho k}|^2) \times \exp\,[-|K_{\rho k}|^2]. \tag{34b}$$

We note that, in the case of initial vacuum state, $\langle Q(0) \rangle$ gives the probability of vacuum remaining vacuum which is less than or equal to unity.

It should be remarked that all the above results, concerning the expectation values with the replacement of K by ζ and with no polarization summation, give the relevant quantities for the case

[5] F. Bloch and A. Nordsiek, Phys. Rev. **52**, 54 (1937).
[6] R. J. Glauber, Phys. Rev. **84**, 395 (1951).

of the neutral scalar meson discussed in the preceding section.

IV. PAIR PRODUCTION OF CHARGED MESONS IN THE PRESENCE OF AN EXTERNAL ELECTROMAGNETIC FIELD

The Lagrange function for the charged meson field, ϕ and $\phi^\dagger$, coupled to an external electromagnetic field potential A and external sources ζ and $\zeta^\dagger$ is given by

$$L(x) = -(i/2)\{\pi_\mu^\dagger, (-i\,\partial_\mu - eA_\mu)\phi\} + \tfrac{1}{4}\{\pi_\mu, \pi_\mu\} - (\mu^2/4)\{\phi, \phi^\dagger\} + \tfrac{1}{2}\{\phi, \zeta\} + \text{H.c.},$$

where H.c. means Hermitian conjugate. By the application of the action principle, the equations of motion are

$$\begin{aligned} i(-i\,\partial_\mu - eA_\mu)\phi &= \pi_\mu, \\ -i(-i\,\partial_\mu - eA_\mu)\pi_\mu &= -\mu^2\phi + \zeta, \\ &+ \text{H.c.}, \end{aligned} \tag{35}$$

and the generators are

$$G_\phi = -\int d\sigma_\mu(\pi_\mu^\dagger\,\delta\phi + \pi_\mu\,\delta\phi^\dagger),$$

$$G_\pi = \int d\sigma_\mu(\delta\pi_\mu^\dagger\phi + \delta\pi_\mu\phi^\dagger).$$

As before, we have

$$\begin{aligned} i\,\partial_0\phi^{(*)} &= \pm\mathcal{E}\phi^{(*)}, \\ \phi^{(*)\dagger} &= \phi^{\dagger(*)}, \\ &+ \text{H.c.}, \end{aligned}$$

$\phi^{(*)}$ representing the positive and negative frequency parts of the field ϕ. The transformation function, $\langle\phi^{(-)'}\phi^{\dagger(-)'}\sigma_1 \mid \phi^{(+)'}\phi^{\dagger(+)'}\sigma_2\rangle$ is given by

$$\langle\phi^{(-)'}\phi^{\dagger(-)'}\sigma_1 \mid \phi^{(+)'}\phi^{\dagger(+)'}\sigma_2\rangle = \exp\Big[\sum_p e^{ipx}\phi_p^{(-)'}\phi^{\dagger(-)'}\phi^{(+)'}\phi^{\dagger(+)'}\Big], \tag{36}$$

where

$$\phi_p^{(+)} = 2\int_{\sigma_2} d\sigma\phi^{(+)}(x)\,\mathcal{E}\phi_p^*(x)e^{ipx_2},$$

$$\phi_p^{(-)} = 2\int_{\sigma_1} d\sigma\phi^{(-)}(x)\,\mathcal{E}\phi_p(x)e^{-ipx_1},$$

$$\phi_p^{\dagger(+)} = 2\int_{\sigma_1} d\sigma\phi^{\dagger(+)}(x)\,\mathcal{E}\phi_p^*(x)e^{-ipx_1},$$

$$\phi_p^{\dagger(-)} = 2\int_{\sigma_2} d\sigma\phi^{\dagger(-)}(x)\,\mathcal{E}\phi_p(x)e^{ipx_2},$$

where

$$\phi_p(x) = \left(\frac{d^3p}{(2\pi)^3}\frac{1}{2\mathcal{E}_p}\right)^{1/2} e^{ipx}.$$

To make the frequency character of ϕ_p's of the above equations more explicit and also for the ease of writing them, we shall define

$$\phi_p^{(-)} = a_{-p}^{(-)}; \quad \phi_p^{(+)} = a_{+p}^{(+)};$$
$$\phi_p^{\dagger(+)} = a_{-p}^{(+)}; \quad \phi_p^{\dagger(-)} = a_{+p}^{(-)};$$

and

$$\phi_{+p}^*(x) = \phi_{-p}(x) = \phi_p^*(x),$$
$$\phi_{-p}^*(x) = \phi_{+p}(x) = \phi_p(x).$$

Then we can write

$$\phi'(x) = \sum_{+p} a_{\lambda p}^{(+)'}\phi_{\lambda p}e^{-ipx_2} + \sum_{-p} a_{\lambda p}^{(-)'}\phi_{\lambda p}^*(x)e^{ipx_1},$$
$$\phi^{\dagger'}(x) = \sum_{+p} a_{\lambda p}^{(-)'}\phi_{\lambda p}^*e^{ipx_1} + \sum_{-p} a_{\lambda p}^{(+)'}\phi_{\lambda p}(x)e^{-ipx_2}.$$

Making use of (36), the projection operator for a state having n charged meson pairs is found:

$$P_n = \prod_{\lambda p}\frac{(a_{\lambda p}^{(-)})^{n\lambda p}}{(n_{\lambda p}!)^{1/2}}\exp\Big[-\sum_p a_{\lambda p}^{(-)}; a_{\lambda p}^{(+)}\Big]\frac{(a_{\lambda p}^{(+)})^{n\lambda p}}{(n_{\lambda p}!)^{1/2}}. \tag{37a}$$

The generating function of the projection operators is given by

$$Q(\lambda) = \exp\Big[(\lambda - 1)\sum_{\lambda p} a_{\lambda p}^{(-)}; a_{\lambda p}^{(+)}\Big] \tag{37b}$$

The field equations for $\langle\phi\rangle$ and $\langle\phi^\dagger\rangle$ in the absence of the external electromagnetic field, but in the presence of the sources ζ and $\zeta^\dagger$ [from Eq. (35)], are

$$[(-i\,\partial_\mu)^2 + \mu^2]\langle\phi\rangle = \zeta$$
$$[(-i\,\partial_\mu)^2 + \mu^2]\langle\phi^\dagger\rangle = \zeta^\dagger$$

The corresponding equation for Green's function is

$$[(-i\,\partial_\mu)^2 + \mu^2]G_0(xx') = \delta(x - x').$$

The various Green's functions we need are given by

$$\begin{aligned} G_0^a(xx') &= -i(S^{(+)} - S^{(-)})(xx')\eta_-(xx'), \\ G_0^r(xx') &= i(S^{(+)} - S^{(-)})(xx')\eta_+(xx'), \\ G_0^{(+)}(xx') &= iS^{(+)}(xx')\eta_+(xx') + iS^{(-)}(xx')\eta_-(xx'), \\ G_0^{(-)}(xx') &= -iS^{(+)}(xx')\eta_-(xx') - iS^{(-)}(xx')\eta_+(xx'), \end{aligned}$$

where

$$S^{(+)}(xx') = \sum_{+\lambda}\phi_{\lambda p}(x)\phi_{\lambda p}^*(x'),$$
$$S^{(-)}(xx') = \sum_{-\lambda}\phi_{\lambda p}(x)\phi_{\lambda p}^*(x').$$

When the external electromagnetic field is present, the equation for Green's function is

$$[(-i\,\partial_\mu - eA_\mu)^2 + \mu^2]G(xx') = \delta(x - x').$$

We define the interaction operator I^i by

$$G^i = G_0^i + G_0^i I^i G_0^i,$$

$$I^i = [e(pA + Ap) - e^2A^2] \times [1 - G_0^i\{e(pA + Ap) - e^2A^2\}]^{-1}$$

The boundary conditions the fields have to satisfy are

$$\begin{aligned}
&\text{(i)} \quad (\phi_- - \phi_+)(x) = 0, \quad \text{for} \quad t \geq t_1 \\
&\qquad + \text{H.c.}; \\
&\text{(ii)} \quad \phi_-(x) = 0 = \phi_+(x), \quad \text{for} \quad t < t_2 \\
&\qquad + \text{H.c.} \\
&\text{(iii)} \quad (\phi_- + \phi_+)(x_2) = \epsilon(\lambda) \coth \tfrac{1}{2}\beta\mathcal{E}(\phi_- - \phi_+)(x_2) \\
&\qquad (\phi_-^\dagger + \phi_+^\dagger)(x_2) = \epsilon(-\lambda) \coth \tfrac{1}{2}\beta\mathcal{E}(\phi_-^\dagger - \phi_+^\dagger)(x_2)
\end{aligned} \tag{38}$$

Hence the required solutions are given by

$$\begin{aligned}
(\phi_- - \phi_+)(x) &= \int_{\sigma_1}^{\sigma_2} d^4x' G^a(xx')(\zeta_- - \zeta_+)(x'), \\
(\phi_-^\dagger - \phi_+^\dagger)(x) &= \int_{\sigma_1}^{\sigma_2} d^4x' (\zeta_-^\dagger - \zeta_+^\dagger)(x') G^r(x'x), \\
(\phi_- + \phi_+)(x) &= \int_{\sigma_2}^{\sigma_1} d^4x' G^r(xx')(\zeta_- + \zeta_+)(x') \\
&\quad + \int_{\sigma_2}^{\sigma_1} d^4x' W_\theta(xx')(\zeta_- - \zeta_+)(x'), \\
(\phi_-^\dagger + \phi_+^\dagger)(x) &= \int_{\sigma_2}^{\sigma_1} d^4x' (\zeta_-^\dagger + \zeta_+^\dagger)(x') G^a(x'x) \\
&\quad + \int_{\sigma_2}^{\sigma_1} d^4x' (\zeta_-^\dagger - \zeta_+^\dagger)(x') W_\theta(x'x),
\end{aligned} \tag{39}$$

where

$$W_\theta(xx') = -\int_{\sigma_2} d\sigma G^r(xx_2) \cdot \frac{\partial}{\partial x_{20}} \times \left[(P^{(+)} - P^{(-)}) \coth \frac{\beta\mathcal{E}}{2} G^a(x_2x')\right].$$

Now the differential characterization of the transformation function is given by

$$\begin{aligned}
\delta\langle|\rangle_\theta^{\sigma_1} &= i\left\langle\left|\int \delta\zeta_+^\dagger\phi_+ + \phi_+^\dagger\,\delta\zeta_+ \right.\right. \\
&\qquad \left.\left. - \delta\zeta_-^\dagger\phi_- - \phi_-^\dagger\,\delta\zeta_-\right|\right\rangle_\theta^{\sigma_1}, \\
&= -\frac{i}{2}\left\langle\left|\int \delta(\zeta_-^\dagger - \zeta_+^\dagger)(\phi_- + \phi_+) \right.\right. \\
&\qquad + \delta(\zeta_-^\dagger - \zeta_+^\dagger)(\phi_- - \phi_+) \\
&\qquad + (\phi_-^\dagger + \phi_+^\dagger)\,\delta(\zeta_- - \zeta_+) \\
&\qquad \left.\left. + (\phi_-^\dagger - \phi_+^\dagger)\,\delta(\zeta_- - \zeta_+)\right|\right\rangle_\theta.
\end{aligned}$$

Using (39), we have

$$\begin{aligned}
\delta\langle|\rangle_\theta^{\sigma_1} = -\frac{i}{2}\left\langle\left|\int \right.\right. &\delta[(\zeta_-^\dagger - \zeta_+^\dagger)(x)G^r(xx')(\zeta_- + \zeta_+)(x') \\
&+ (\zeta_-^\dagger + \zeta_+^\dagger)(x)G^a(xx')(\zeta_- - \zeta_+)(x') \\
&\left.\left. + (\zeta_-^\dagger - \zeta_+^\dagger)(x)W_\theta(xx')(\zeta_- - \zeta_+)(x')\right|\right\rangle_\theta.
\end{aligned}$$

The functional integration gives

$$\langle\sigma_2 \mid \sigma_2\rangle_\theta^{\sigma_1} = \exp[i\zeta^\dagger G_\theta \zeta], \tag{40}$$

where

$$G_\theta = -\frac{1}{2}\begin{pmatrix} -G^a - G^r + W_\theta & G^a - G^r - W_\theta \\ -G^a + G^r - W_\theta & G^a + G^r + W_\theta \end{pmatrix},$$

and

$$\zeta^\dagger = \overbrace{\zeta_+^\dagger \quad \zeta_-^\dagger}; \qquad \zeta = \begin{pmatrix} \zeta_+ \\ \zeta_- \end{pmatrix}.$$

Let us evaluate $\langle Q(\lambda)\rangle$ of (37b). We shall confine ourselves to the case of vacuum ($\beta \to \infty$). Let us introduce

$$\begin{aligned}
\nu(x) &= \sum_{\lambda p} \nu_{\lambda p}\phi_{\lambda p}(x), \\
\nu^*(x) &= \sum_{\lambda p} \nu_{\lambda p}^*\phi_{\lambda p}(x).
\end{aligned}$$

Then $\langle Q(\lambda)\rangle$ can be written as

$$\langle Q(\lambda)\rangle = \prod_{\lambda p} \exp\left[-(\lambda - 1)\frac{\partial}{\partial\nu_{\lambda p}}\frac{\partial}{\partial\nu_{\lambda p}^*}\right] \times \langle(\exp i[\nu^\dagger\mathcal{E}\phi + \nu\mathcal{E}\phi^\dagger])_+\rangle|_{\nu^\dagger=0=\nu}, \tag{41}$$

where the time ordering refers to the fact that ν_{+p} and $\nu_{-p}^\dagger$ are later than $\nu_{+p}^\dagger$ and ν_{-p} in the limit as we reach the surface σ_1, where $\langle Q(\lambda)\rangle$ is evaluated. In order to generate $(\ )_+$ in Eq. (41), we let

$$\begin{aligned}
&\zeta_+^\dagger(x) \to \zeta_+^\dagger(x) \\
&\quad + \nu^\dagger(x)(P^{(+)}\,\delta(t - t_1) + P^{(-)}\,\delta(t - t_1 - 0))\mathcal{E}, \\
&\zeta_+(x) \to \zeta_+(x) \\
&\quad + \mathcal{E}(P^{(+)}\,\delta(t - t_1 - 0) + P^{(-)}\,\delta(t - t_1))\nu(x),
\end{aligned}$$

and let the sources ζ_- and $\zeta_+^\dagger$ equal to zero. Then

$$\begin{aligned}
\langle Q(\lambda)\rangle = \prod_{\lambda p} &\exp\left[-(\lambda - 1)\frac{\partial}{\partial\nu_{\lambda p}}\frac{\partial}{\partial\nu_{\lambda p}^*}\right] \\
&\times \exp i\left[\int \nu^\dagger(P^{(+)}\,\delta(t - t_1) + P^{(-)}\,\delta(t - t_1 - 0)) \right. \\
&\times \mathcal{E}G_{++}\mathcal{E}(P^{(+)}\,\delta(t - t_1 - 0) \\
&\left. + P^{(-)}\,\delta(t - t_1)\nu\right]\Big|_{\nu^\dagger=0=\nu}.
\end{aligned} \tag{42a}$$

Now

$$G_{++} = \tfrac{1}{2}(2G_0^{(+)} + G_0^a I^a G_0^a + G_0^r I^r G_0^r - W_I) \qquad (42b)$$

When the surface σ_1 is approached in Eq. (42a), all the terms except W_I on the right of Eq. (42b) give vanishing contribution. The entire contribution comes from

$$-\tfrac{1}{2}W_I = \frac{1}{2}\int_{\sigma_2} d\sigma\Big\{G_0^r(xx_2)\cdot\frac{\partial}{\partial x_{20}}(P^{(+)} - P^{(-)})G_0^a I^a G_0^a + G_0^r I^r G_0^r(xx_2)\cdot(\partial/\partial x_{20})(P^{(+)} - P^{(-)})G_0^a + G_0^r I^r G_0^r(xx_2)\cdot(\partial/\partial x_{20})(P^{(+)} - P^{(-)})G_0^a I^a G_0^a\Big\}.$$

Using

$$\int_{\sigma_2} d\sigma G_0^r(xx_2)\cdot\frac{\partial}{\partial x_{20}}(P^{(+)} - P^{(-)})G_0^a(x_2x') = i\sum_{\lambda p}\phi_{\lambda p}(x)\phi_{\lambda p}^*(x') = i(S^{(+)} + S^{(-)})(xx'),$$

$$\tfrac{1}{2}W_I = \tfrac{1}{2}[(S^{(+)} - S^{(-)})I^r(S^{(+)} + S^{(-)}) - (S^{(+)} + S^{(-)})I^a(S^{(+)} - S^{(-)}) + i(S^{(+)} - S^{(-)})I^r(S^{(+)} + S^{(-)})I^a(S^{(+)} - S^{(-)})].$$

The last exponent in Eq. (42a) becomes

$$\int\nu^\dagger\cdots\varepsilon G_{++}\varepsilon\cdots\nu = -\tfrac{1}{2}\nu^\dagger[ig^a\mathfrak{A} - i\mathfrak{A}g^r + \mathfrak{A}g^r g^a\mathfrak{A}]\nu,$$

where g^r, g^a and $\mathfrak{A}$ are, respectively, I^r, I^a and $(S^{(+)} - S^{(-)})$ in the λp representation. Hence,

$$\langle Q(\lambda)\rangle = \exp\left[-(\lambda - 1)\frac{\partial}{\partial\nu}\frac{\partial}{\partial\nu^\dagger}\right] \times \exp\left[-\tfrac{1}{2}\nu^\dagger(ig^a\mathfrak{A} - i\mathfrak{A}g^r + \mathfrak{A}g^r g^a\mathfrak{A})\nu\right]\Big|_{\nu^\dagger=0=\nu}$$
$$= \det{}^{-1}[1 - \tfrac{1}{2}(\lambda - 1)(ig^a\mathfrak{A} - i\mathfrak{A}g^r + \mathfrak{A}g^r g^a\mathfrak{A})].$$

Using the identity

$$g^r - g^a = ig^r\mathfrak{A}g^a,$$

and after some algebraic manipulations, we get

$$\langle Q(\lambda)\rangle = \det{}^{-1}[1 - (\lambda - 1)I^r S^{(-)}I^a S^{(+)}]. \qquad (43)$$

Using the identities

$$I^r = (1 - iI^{(-)}S^{(+)})I^{(-)},$$
$$I^a = (1 + iI^{(+)}S^{(+)})I^{(+)},$$

and

$$I^{(+)} - I^{(-)} = iI^{(+)}(S^{(+)} + S^{(-)})I^{(-)},$$

we get

$$(1 + iI^r S^{(+)})(1 - iS^{(+)}) = 1 + I^r S^{(-)}I^a S^{(+)} = (1 - I^{(+)}S^{(-)}I^{(-)}S^{(+)})^{-1}.$$

Hence

$$\langle Q(\lambda)\rangle = \det{}^{-1}[1 - (\lambda - 1)I^r S^{(-)}I^a S^{(+)}]$$
$$= \det{}^{-1}[\lambda - (\lambda - 1)(1 + I^r S^{(-)}I^a S^{(+)})]$$
$$= \det\left(\frac{1 - I^{(+)}S^{(-)}I^{(-)}S^{(+)}}{1 - \lambda I^{(+)}S^{(-)}I^{(-)}S^{(+)}}\right) \qquad (44)$$

We have $\langle Q(1)\rangle = 1$, illustrating completeness trivially; and

$$\langle Q(0)\rangle = \det(1 - I^{(+)}S^{(-)}I^{(-)}S^{(+)})$$

is the probability that vacuum remains vacuum and is less than or equal to unity as

$$I_{(+-)}^{(-)} = I_{(+-)}^{(+)*}; \qquad I_{(-+)}^{(-)} = I_{(-+)}^{(+)*}$$

and hence, $I_{(-+)}^{(+)}I_{(+-)}^{(-)}$ and $I_{(+-)}^{+}I_{(-+)}^{(-)}$ are non-negative Hermitian matrices which possess non-negative, real eigenvalues. $p(n, 0)$, the probability that n charged meson pairs are produced with the initial vacuum state, is given by extracting the coefficient of λ^n in (44):

$$p(n, 0) = \det(1 - I^{(+)}S^{(-)}I^{(-)}S^{(+)}) \times\frac{1}{n!}\int dx_1\cdots dx_n perm_{(n)} \times\langle x_i\,|I^{(+)}S^{(-)}I^{(-)}S^{(+)}|\,x_j\rangle. \qquad (45)$$

V. PAIR PRODUCTION OF FERMIONS IN THE PRESENCE OF AN EXTERNAL ELECTROMAGNETIC FIELD

This case is similar to the case of pair production of charged mesons treated in the preceding section, but there is one very important difference. Instead of condition (iii) of Eq. (38), we have

$$(\psi_- + \psi_+)(x_2) = \epsilon(\lambda)\tanh\tfrac{1}{2}\beta\,\varepsilon(\psi_- - \psi_+)(x_2),$$

ψ being the fermion field. This happens to be the case because the fermion sources are the elements of the Grassmann exterior algebra.[7] The evaluation of $\langle Q(\lambda)\rangle$ in this case gives

$$\langle Q(\lambda)\rangle = \det\left[\frac{1 + \lambda I^{(+)}S^{(-)}I^{(-)}S^{(+)}}{1 + I^{(+)}S^{(-)}I^{(-)}S^{(+)}}\right],$$

$$p(n, 0) = \det{}^{-1}[1 + I^{(+)}S^{(-)}I^{(-)}S^{(+)}] \times\frac{1}{n!}\int dx_1\cdots dx_n\det{}_{(n)} \times\langle x_i\,|I^{(+)}S^{(-)}I^{(-)}S^{(+)}|\,x_j\rangle, \qquad (46)$$

where

[7] J. Schwinger, Lectures delivered at the University of California at Los Angeles, spring of 1961, (unpublished); Proc. Natl. Acad. Sci. U. S. 48, 603 (1962).

$$S^{(+)}(xx') = \sum_{+p} \psi_{\lambda p}(x)\bar{\psi}_{\lambda p}(x'),$$
$$S^{(-)}(xx') = \sum_{-p} \psi_{\lambda p}(x)\bar{\psi}_{\lambda p}(x'), \tag{47b}$$

where

$$\psi_{\lambda p}(x) = \left(\frac{d^3p}{(2\pi)^3}\frac{m}{p_0}\right)^{1/2} u_{\lambda p} e^{i\epsilon(\lambda)px},$$

where

$$\epsilon(\lambda) = \lambda/|\lambda|, \qquad \lambda = \pm 1, \pm 2,$$

and $u_{\lambda p}$ satisfies the equation

$$[\gamma p + \epsilon(\lambda)m]u_{\lambda p} = 0. \tag{47b}$$

We have also

$$\int_\sigma d\sigma \bar{\psi}_{\lambda p}\gamma_0\psi_{\lambda p} = \delta_{\lambda p,\lambda' p'}.$$

$I^{(*)}$ is given by

$$I^{(*)} = e\gamma A(1 - G_0^{(*)}e\gamma A)^{-1} \tag{47c}$$

where

$$G_0^{(*)} = \pm iS^{(+)}(xx')\eta_*(xx') \mp iS^{(-)}(xx')\eta_*(xx').$$

Equation (46) was obtained by Salam and Mathews[8] and Schwinger.[2]

ACKNOWLEDGMENT

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[8] A. Salam and P. T. Mathews, Phys. Rev. 90, 690 (1953).

Expectation Value Formalism in Quantum Field Theory. II

PRADIP M. BAKSHI AND KALYANA T. MAHANTHAPPA*†
Lyman Laboratories, Harvard University, Cambridge, Massachusetts
(Received 18 May 1962)

The expectation value formalism has been developed to treat the problems which require the coupling of quantized Fermi and Bose fields.

I. INTRODUCTION

IN the preceding paper,[1] we have considered the quantized Fermi and Bose fields in the presence of external sources and an external electromagnetic field. To deal with physically meaningful problems of field theory, one has to consider the coupled system of quantized Fermi and Bose fields. Generation of the expectation values of the projection operators of the physical quantities of interest in this case requires not only the introduction of "plus" and "minus" sources for each of the fields, but also "plus" and "minus" external Bose fields. In what follows, though we refer to quantum electrodynamics in particular, the treatment of the problem has general applicability.

In the next section, we take up the study of the general structure of the required transformation function. In Sec. III, we construct the transformation for the electron field coupled to sources $\eta_\pm(x)$ and external electromagnetic fields with potentials $A_\pm^e(x)$. Section IV concerns the application of the formalism to evaluate the expectation values of projection operators and, in particular, that of $Q(\lambda)$ of Sec. III of I.

II. GENERAL STRUCTURE OF $\langle 0\sigma_2 \mid 0\sigma_2 \rangle^\pm$

The Lagrange function which describes the interacting electron and electromagnetic fields in the presence of an external electromagnetic field and external sources is given by

$$L(x) = -\tfrac{1}{2}[\bar{\psi}, \gamma_\mu(-i\,\partial_\mu - eA_\mu^e)\psi + m\psi] + \bar{\psi}\eta + \eta\psi + \tfrac{1}{4}F_{\mu\nu}^2 - \tfrac{1}{2}F_{\mu\nu}(\partial_\mu A_\nu - \partial_\nu A_\mu) + K_\mu A_\mu + e\bar{\psi}\gamma_\mu A_\mu\psi, \quad (1)$$

where ψ and $\bar{\psi}$ denote the electron field, A_μ the electromagnetic potential, A_μ^e a prescribed external electromagnetic potential, η and $\bar{\eta}$ prescribed sources of electron field, and K_μ a prescribed external current distribution. In the expression (1), symmetrized and antisymmetrized multiplication is to be understood for Bose and Fermi fields, respectively. We shall refer to the first terms of (1) as L_e, the Lagrange function for an electron field interacting with external quantities η and $\bar{\eta}$ and A_μ^e; the last term as L_c, which represents the coupling between electron and electromagnetic fields; the rest of the terms as L_{em}. The following development is independent of the particular structure of L_e and L_{em}, and depends on the locality of L_c. If it is desired to increase the number of components of a particular field, it can be done by replacing charge by a matrix and interpreting scalar products as those in higher dimension in which the field would be.

Now our object is to obtain the transformation function $\langle 0\sigma_2 \mid 0\sigma_2\rangle^*$ when all the external quantities have the "plus" characterization in the forward development in time and the "minus" characterization in the backward development.[1] The differential characterization of the function $\langle 0\sigma_2 \mid 0\sigma_2\rangle^*$ is provided by the extension of the action principle:

$$\delta\langle 0\sigma_2 \mid 0\sigma_2\rangle^* = i\langle 0\sigma_2 \mid \delta W_+ - \delta W_- \mid 0\sigma_2\rangle^*, \quad (2)$$

where the action operators $W_\pm$ are given by

$$W_\pm = \int_{\sigma_2}^{\sigma_1} d^4x L_\pm(x),$$

σ_1 being the later surface at which measurements are made. We shall integrate Eq. (2) as follows.[2] Let

$$L_\pm = L_{\pm em} + L_{\pm e} + \lambda_\pm L_{\pm c},$$

and let the parameters $\lambda_\pm$ vary from zero to unity. The purpose of introducing $\lambda_\pm$ is to express the coupling of the electron and electromagnetic fields in terms of their coupling to external quantities. The variation of $\lambda_\pm$ yields

* Work done while a Faculty of Arts and Sciences Fellow, Harvard University (1960–1961).

† Present address: Department of Physics, University of California, Los Angeles, California.

[1] P. M. Bakshi and K. T. Mahanthappa, preceding paper, J. Math. Phys. 4, 1 (1963). This paper will be referred to as I.

[2] J. Schwinger, "Lectures on the Theory of Coupled Fields, Harvard University, 1954" (unpublished). A parameter λ was used to get an expression for $\langle 0\sigma_1 \mid 0\sigma_2\rangle$.

$$\delta_{\lambda_\pm}\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = i\left\langle\left|\int \delta\lambda_+ L_{+c} - \delta\lambda_- L_{-c}\right|\right\rangle^\pm. \quad (3a)$$

This can be written as

$$\pm(1/i)(\delta/\delta\lambda_\pm)\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = \langle|L_{\pm c}|\rangle. \quad (3b)$$

Note that $\pm$ in $\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm$ refers to notation only. The variations of external quantities yield

$$\pm(1/i)(\delta/\delta K_\pm)\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = \langle|A_\pm|\rangle, \quad (3c)$$

$$\pm(1/i)(\delta/\delta\eta_\pm)\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = \langle|\bar{\psi}_\pm|\rangle, \quad (3d)$$

$$\pm(1/i)(\delta/\delta\bar{\eta}_\pm)\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = \langle|\psi_\pm|\rangle. \quad (3e)$$

Note that the variations as represented by (3c) are restricted to the class $\partial_\mu\, \delta K_\mu(x) = 0$. That is, $A_\mu(x)$ is arbitrary to the extent of containing a gradient of a scalar with no change in variation of the transformation function. This is a consequence of gauge invariance of the electromagnetic field. Using Eqs. (3) and the fact that $L_c = j_\mu A_\mu$ (where $j_\mu = e\bar{\psi}\gamma_\mu\psi$):

$$(\delta^2/\delta A_\pm^e\, \delta K_\pm)\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = -\langle|j_\pm A_\pm|\rangle^\pm = \mp i(\delta/\delta\lambda_\pm)\langle|\rangle^\pm.$$

Carrying out the functional integrations and setting $\lambda_+ = 1 = \lambda_-$, we get

$$\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = \exp\left[-i\int\left(\frac{\delta}{\delta A_+^e}\frac{\delta}{\delta K_+} - \frac{\delta}{\delta A_-^e}\frac{\delta}{\delta K_-}\right)\right] \times \langle 0\sigma_2 \mid 0\sigma_2\rangle_{e+em}^\pm, \quad (4a)$$

where $\langle 0\sigma_2 \mid 0\sigma_2\rangle_{e+em}^\pm$ refers to uncoupled fields and is given by

$$\langle 0\sigma_2 \mid 0\sigma_2\rangle_{e+em}^\pm = \langle 0\sigma_2 \mid 0\sigma_2\rangle_e^\pm \langle 0\sigma_2 \mid 0\sigma_2\rangle_{em}^\pm. \quad (4b)$$

The function $\langle 0\sigma_2 \mid 0\sigma_2\rangle_{em}^\pm$ is given by the Eq. (29) of the preceding paper[1] with $\beta \to \infty$. To obtain an expression for $\langle 0\sigma_2 \mid 0\sigma_2\rangle_e^\pm$, the transformation function with the Lagrange function $L_{\pm e}$, will be the subject matter of the next section. Now, using the identity

$$\exp\,[C\ \delta/\delta A_\pm^e]F(A_\pm^e) = F(C + A_\pm^e),$$

we have for (4a), explicitly indicating the functional dependences,

$$\langle 0\sigma_2 \mid 0\sigma_2\rangle^\pm = \langle 0\sigma_2 \mid 0\sigma_2\rangle_e^\pm(\eta_\pm, \bar{\eta}_\pm, A_\pm^e \pm (1/i)\ \delta/\delta K_\pm) \times \langle 0\sigma_2 \mid 0\sigma_2\rangle_{em}^\pm(K_\pm). \quad (5)$$

III. CONSTRUCTION OF $\langle\, 0\sigma_2/0\sigma_2\,\rangle_e^\pm$

We could follow the same procedure as in I and express $\langle 0\sigma_2 \mid 0\sigma_2\rangle_e^\pm$ in terms of the retarded and advanced Green's functions. Though the expression one would get this way expresses causality and the unitary nature of the theory explicitly, it is not easily amenable to computation. Hence we shall adopt another way which gives the required transformation function in terms of $G^{(+)}$ and $G^{(-)}$, the causal and anticausal Green's functions of the electron field in the presence of an external electromagnetic field. Because there is no confusion, we shall indicate A^e by A. Then we have

$$(\gamma p + m - e\gamma A)G^{(\pm)} = 1. \quad (6)$$

The construction of the transformation function is achieved by the operation of time reflection and a phase transformation on the regular transformation function[2] $\langle 0\sigma_1 0\sigma_2\rangle_*$. Though the n-electron and m-photon interacting Green's functions $G_p^{(+)}$ and $G_p^{(-)}$ satisfy intrinsically different sets of differential equations, Schwinger[3] has shown, by analytical continuation, that

$$G_p^{(-)}(x) = (-1)^n G_p^{(+)}(-e^{-\pi i}x). \quad (7)$$

We shall understand the significance of this operation by looking at the differential equation that $G_p^{(+)}$ satisfies:

$$(\gamma_\mu\,\partial_\mu + im)G_p^{(+)}(x_1 \cdots x_{2p}) + \cdots = i\,\delta(x_1 - x_2)G_{p-1}^{(+)}(x_3 \cdots x_{2p}) \pm i\,\delta(x - x_3)G_{p-1}^{(+)}(x_2 \cdots x_{2p}) \pm \cdots. \quad (8)$$

The other terms on the left are combinations of Green's functions that are necessary to represent the interacting effects in the field equations. The corresponding equation for $G_p^{(-)}$ has the left side the same as (8), but differs on the right in the sign of i exhibited by photon terms. The effect of the transformation (7) to get the equation for $G_p^{(-)}$ from (8) can be interpreted as follows: Operation of $-e^{-\pi i}$ on the space coordinates means multiplication by unity; the operation on time coordinates has to be viewed in two stages, (i) time reflection reverses the time ordering and (ii) multiplication by $e^{-\pi i}$ retains the time ordering but changes the sign of time coordinates. Thus, under $-e^{-\pi i}$ operation, $\delta(t - t') \to -(t - t')$. $(-1)^n$ in (7) reverses the sign of electron terms on the right side of (8).

Thus, under the operation of $-e^{-\pi i}$, we have

$$A(x) \to A(x),$$
$$G^{(+)}(x) \to -G^{(-)}(x),$$
$$\eta(x) \to \eta(x).$$

[3] J. Schwinger, Phys. Rev. **115**, 721 (1959); *Ninth Annual International Conference on High Energy Physics, Kiev, 1959* (Academy of Sciences, U. S. S. R., 1960).

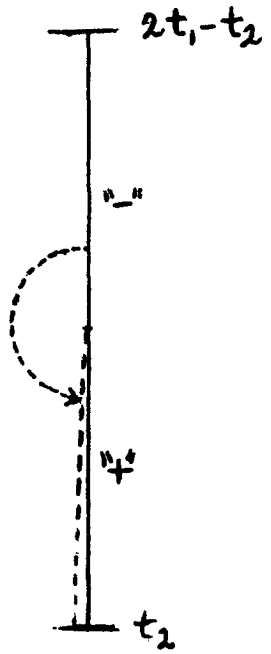

FIG. 1.

In the matrix notation,

$$\begin{aligned}\langle x\,|A|\,x'\rangle &\to -\langle x\,|A|\,x'\rangle,\\ \langle x\,|G|\,x'\rangle &\to \langle x\,|G|\,x'\rangle,\\ \langle x\,|\eta|\,x'\rangle &\to -\langle x\,|\eta|\,x'\rangle.\end{aligned}\tag{9}$$

As a simple example of (9), we have

$$\det(1 - e\gamma AG_0^{(+)}) \to \det(1 + e\gamma AG_0^{(-)}) = \det(1 - e\gamma AG_0^{(-)})$$

as the determinant here is an even function of e. Now we shall carry out this operation of the transformation function $\langle 2\sigma_1 - \sigma_2 \mid \sigma_2\rangle$ (which is an expression of the fact that we are concerned with the time interval from t_2 to $(2t_1 - t_2)$) to get $\langle 0\sigma_2 \mid 0\sigma_2\rangle_e^*$. To do this, divide the region in time into two equal intervals of $t_1 - t_2$ (see Fig. 1); apply the transformation on the later interval symbolizing the external quantities in that region by "$-$" subscript; the resultant expression is $\langle 0\sigma_2 \mid 0\sigma_2\rangle_e^*$. Now

$$\langle 2\sigma_1 - \sigma_2 \mid \sigma_2\rangle = \det(1 - e\gamma AG_0^{(+)}) \exp[i\bar{\eta}G^{(+)}\eta].\tag{10}$$

We shall split all the external quantities η, $\bar{\eta}$ and A as $\eta_+ + \eta_-$, $\bar{\eta}_+ + \bar{\eta}_-$ and $A_+ + A_-$ and assume that "plus" quantities exist in the "plus" region and "minus" quantities exist in the "minus" region; we shall not indicate it explicitly by writing step functions. Then (10) becomes

$$\begin{aligned}\langle 2\sigma_1 - \sigma_2 \mid \sigma_2\rangle &= \det[1 - e\gamma(A_+ + A_-)G_0^+]\\ &\times \exp i[\langle x_+\,|\bar{\eta}|\,x'_+\rangle\langle x'_+\,|G^{(+)}|\,x'''_+\rangle\langle x'''_+\,|\eta|\,x'_+\rangle\\ &+ \langle x_+\,|\bar{\eta}|\,x''_+\rangle\langle x''_+\,|G^{(+)}|\,x'''_-\rangle\langle x'''_-\,|\eta|\,x'_-\rangle\\ &+ \langle x_-\,|\bar{\eta}|\,x''_-\rangle\langle x''_-\,|G^{(+)}|\,x'''_-\rangle\langle x'''_-\,|\eta|\,x'_-\rangle\\ &+ \langle x_-\,|\bar{\eta}|\,x''_-\rangle\langle x''_-\,|G^{(+)}|\,x'''_+\rangle\langle x'''_+\,|\eta|\,x'_-\rangle.\end{aligned}$$

Upon transformation

$$\begin{aligned}\langle x_\pm\,|\eta|\,x'_\pm\rangle &\to \pm\eta_\pm,\\ \langle x_\pm\,|G^{(+)}|\,x'_\pm\rangle &\to G_{\pm\pm},\\ \langle x_\pm\,|G^{(+)}|\,x'_\mp\rangle &\to -G_{\pm\mp},\\ \langle x_\pm\,|A|\,x'_\pm\rangle &\to \pm A_\pm.\end{aligned}$$

We shall illustrate how to get the explicit expression for G_{++}. Consider

$$\begin{aligned}\langle x_+\,|G^{(+)}|\,x'_+\rangle &= \langle x_+\,|(1 - G_0^{(+)}e\gamma A)^{-1}G_0^{(+)}|\,x'_+\rangle\\ &= \langle x_+\,|[1 - G_0^{(+)}e\gamma(A_+ + A_-)]^{-1}G_0^{(+)}|\,x_+\rangle\\ &= \left\langle x_+\left|G_0^{(+)}\frac{1}{1 - e\gamma A_-G_0^{(+)}}\left[1 - \frac{1}{1 - e\gamma A_+G_0^{(+)}}\right.\right.\right.\\ &\quad\left.\times e\gamma A_+G_0^{(+)}e\gamma A_-\frac{1}{1 - G_0^+e\gamma A_-}G_0^{(+)}\right]^{-1}\\ &\quad\left.\times\frac{1}{1 - e\gamma A_+G_0^{(+)}}\right|x'_+\right\rangle\end{aligned}$$

$$\xrightarrow{x_-\to -x_-e^{-\pi i}} G_{++}$$

$$\begin{aligned}&= \left(G^0_{++} - G^0_{+-}e\gamma A_-\frac{1}{1 + e\gamma A_-G^0_{--}}G_{-+}\right)\\ &\quad\times\left[1 + \frac{1}{1 - e\gamma A_+G^0_{++}}\right.\\ &\quad\left.\times e\gamma A_+G^0_{+-}e\gamma A_-\frac{1}{1 + G_{--}e\gamma A_-}G_{++}\right]^{-1}\\ &\quad\times[1 - e\gamma A_+G_{++}]^{-1}.\end{aligned}$$

It is easily seen that $G^0_{++} = G_0^{(+)}$, $G^0_{+-} = iS^{(-)}$, $G^0_{-+} = -iS^{(+)}$ and $G^0_{--} = -G_0^{(-)}$, S^+ and S^- being given in Sec. V of I. Hence

$$\begin{aligned}G_{++} &= (G_0^{(+)} - S^{(-)}I_-^{(-)}S^{(+)})\\ &\times(1 + I_+^{(+)}S^{(-)}I_-^{(-)}S^{(+)})^{-1}(1 - e\gamma A_+G_0^{(+)})^{-1},\end{aligned}\tag{11a}$$

where

$$I_\pm^* = e\gamma A_\pm/(1 - G_0^{(*)}e\gamma A_\pm).$$

Similarly, we have

$$G_{\pm\mp} = \pm i(1 - G_0^{(\pm)} e\gamma A_\pm)^{-1} \times S^{(\mp)}(1 + I_\mp^{(\mp)} S^{(+)} I_\pm^{(\pm)} S^{(\mp)})^{-1} \times (1 - e\gamma A_\pm G_0^{(\pm)})^{-1}, \tag{11b}$$

$$G_{--} = -(G_0^{(-)} - S^{(+)} I_+^{(+)} S^{(-)}) \times (1 + I_-^{(-)} S^{(+)} I_+^{(+)} S^{(-)})^{-1} \times (1 - e\gamma A_- G_0^{(-)})^{-1}. \tag{11c}$$

The required transformation function is

$$\langle 0\sigma_2 \mid 0\sigma_2\rangle_e^* = C(A_\pm) \exp [i\bar{\eta} G \eta], \tag{12a}$$

where

$$\bar{\eta} = \overbrace{\bar{\eta}_+ \quad \bar{\eta}_-}; \qquad \eta = \begin{pmatrix} \eta_+ \\ \eta_- \end{pmatrix}$$

$$G = \begin{pmatrix} G_{++} & G_{+-} \\ G_{-+} & G_{--} \end{pmatrix} \tag{12b}$$

and $C(A_\pm)$ is the transform of the determinant in (10) and is given by

$$C(A_\pm) = \det (1 - e\gamma A_+ G_0^{(+)}) \det (1 - e\gamma A_- G_0^{-}) \times \det [1 + I_+^{(+)} S^{(-)} I_-^{(-)} S^{(+)}]. \tag{12c}$$

IV. EXPECTATION VALUE OF Q (λ)

The complete transformation function, using Eqs. (29) of I, (5), and (12), is

$$\langle 0\sigma_2 \mid 0\sigma_2\rangle^* = C\left(A_\pm^e \pm \frac{1}{i}\frac{\delta}{\delta K_\pm}\right) \times \exp\left[i\bar{\eta} G\left(A_\pm^e \pm \frac{1}{i}\frac{\delta}{\delta K_\pm}\right)\eta\right] \times \exp (\tfrac{1}{2} iKDK). \tag{13}$$

This transformation function contains all the physical information of the coupled system of quantized electron and electromagnetic fields. We can generate the expectation values directly by appropriate operations. As an example, consider evaluation of the expectation value of $Q(\lambda)$ of Eq. (24b) of I. Proceeding as before, we get from Eq. (32a) of I, and (13),

$$\langle Q(\lambda)\rangle = C \exp [i\bar{\eta} G \eta] \exp [\tfrac{1}{2} iKDK] \times \exp [(\lambda - 1)K_+ SK_-] \mid_{K_+=0=K_-}. \tag{14}$$

K_+ and K_- are equated to zero only after all the operations of variational differentation are carried out. From (14), we can generate the cross section for n-photon production in any process in quantum electrodynamics, provided we know the elements of G explicitly.

As particular examples, we shall explicitly write down the matrix elements one needs to evaluate in multiple production of photons in pair annihilation and Coulomb scattering. The matrix element for the case of pair annihilation is

$$\langle t_2; 1_{+p} 1_{-p'} \mid Q(t; \lambda) \mid 1_{+p} 1_{-p'}; t_2'\rangle, \tag{15a}$$

where p and p' are the four momenta of electron and positron. Making use of the creation and annihilation operators[4] $\chi_{\lambda p}^{(\pm)}$, (15a) becomes

$$\langle t_2 \mid (\chi_{+p}^{(+)} \chi_{-p'}^{(+)})_{t_2} Q(t; \lambda) (\chi_{-p'}^{(-)} \chi_{+p}^{(-)})_{t_2'} \mid t_2'\rangle = \int (\bar{\psi}_{+p}\gamma_0)_{t_2} (\bar{\psi}_{-p}\gamma_0)_{t_2'} \times \langle t_2 \mid \psi(t_2)\bar{\psi}(t_2) Q(t; \lambda) \psi(t_2')\bar{\psi}(t_2') \mid t_2'\rangle \times (\gamma_0 \psi_{+p})_{t_2'} (\gamma_0 \psi_{-p'})_{t_2}, \tag{15b}$$

where $\psi_{\lambda p}$ and $\bar{\psi}_{\lambda p}$ are given by Eq. (47) of I and the integral sign refers to the integrations over appropriate surfaces. In (15b), the transition from the free-field ψ's to the interacting ψ's is assumed. In other words, the asymptotic condition is assumed. The physical meaning of using the free-field projection operators amounts to saying that all the measurements are carried out in the limit of free fields. By proper variational differentiation of (14) with respect to $\eta_\pm$ and $\bar{\eta}_\pm$, we get

$$\langle t_2 \mid \psi(t_2)\bar{\psi}(t_2) Q(\lambda; t) \psi(t_2')\bar{\psi}(t_2') \mid t_2'\rangle = -CG_{--}(t_2; t_2 + 0) G_{++}(t_2' + 0; t_2') \times \exp (\tfrac{1}{2} iKDK) \exp [(\lambda - 1)K_+ SK_-] \mid_{K_+=0=K_-}.$$

Hence we have

$$\langle t_2; 1_{+p} 1_{-p'} \mid Q(\lambda; t) \mid 1_{+p} 1_{-p'}; t_2\rangle = -C\left[\int \bar{\psi}_{+p}\gamma_0 G_{--} \gamma_0 \psi_{-p'}\right] \times \left[\int \bar{\psi}_{-p'}\gamma_0 G_{++} \gamma_0 \psi_{+p}\right] \times \exp (\tfrac{1}{2} iKDK) \times \exp [(\lambda - 1)K_+ SK_-] \mid_{K_+=0=K_-}. \tag{16}$$

The matrix element for multiple bremsstrahlung is

$$\langle t_2\ 1_{+p} \mid (\chi_{+p'}^{(-)} Q(\lambda) \chi_{+p}^{(+)})_{t_1} \mid 1_{+p}; t_2\rangle, \tag{17}$$

where p and p' are initial and final four momenta of electron. We can write (17) as

[4] J. Schwinger, Phys. Rev. **92**, 1283 (1953).

$$\langle t_2 \,|(\chi^{(+)}_{+p})_{t_2}(\chi^{(-)}_{+p'}Q(\lambda)\chi^{(+)}_{+p'})_{t_1}(\chi^{(-)}_{+p})'_{t'_2}|\, t'_2\rangle$$

$$= \int (\bar{\psi}_{+p}\gamma_0)_{t_2}(\bar{\psi}\gamma_0)_{t_1}\langle t_2 \,|\psi(t_2)\bar{\psi}(t_1)Q\psi(t_1)\bar{\psi}(t'_2)|\, t'_2\rangle$$

$$\times (\gamma_0\psi_{+p'})_{t_1}(\gamma_0\psi_{+p})_{t_2}$$

$$= -C\Big[\int \bar{\psi}_{+p}\gamma_0 G_{--}\gamma_0\psi_{+p'}\Big]\Big[\int \bar{\psi}_{+p'}\gamma_0 G_{++}\gamma_0\psi_{+p}\Big]$$

$$\times \exp[\tfrac{1}{2}iKDK] \exp[(\lambda - 1)K_+SK_-]. \qquad (18)$$

In (16) and (18), we have neglected terms of the structure $(G_{+-})_{pp}(G_{-+})_{p'p'}$ because they represent only vacuum fluctuations and do not correspond to the phenomenon in question.

By the above examples, we see that the problem of evaluating the expectation value of $Q(\lambda)$ in any specific process has reduced to getting explicit expressions for G_{++} and G_{--} which one could do in the framework of an approximation scheme. The simplicity of the expressions (16) and (18) is due to the simple expression we have for $Q(\lambda)$. $Q(\lambda)$ is the generating function for projection operators for n-photon states. The only things specified are the number of photons and their total energy. But if one needed detailed information concerning individual polarization and energy of photons, the expressions would no longer be simple. Thus, the less detailed the information one asks for, the simpler would be the expressions that are to be evaluated. This is in contrast with the evaluation of expectation values using scattering amplitude.

Note added in proof: For an application of the formalism developed in this paper see K. T. Mahanthappa, Phys. Rev. **126**, 329 (1962).

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Relativistic Invariance and the Square-Root Klein-Gordon Equation*

J. SUCHER
Department of Physics, University of Maryland, College Park, Maryland
(Received 2 April 1962)

Although the usual operator invariance requirements and corresponding commutation conditions encountered in the study of the invariance of relativistic wave equations (and other equations of physics) are sufficient conditions for invariance, they are by no means necessary. More general conditions are given and illustrated with the square-root Klein-Gordon equation. A new proof is thereby given of the Lorentz invariance of this equation. The methods developed are extended to cover the presence of external fields, and it is proved that the usual gauge invariant modification of the relativistic Hamiltonian of a spinless particle which takes into account the presence of an external electromagnetic field leads, in the quantum mechanical case, to an equation which does *not* admit the proper Lorentz group. This theorem and its generalization are discussed in connection with Dirac's statement that the square-root equation cannot be extended to include interaction without losing Lorentz invariance.

1. INTRODUCTION

CONSIDER an equation of the form

$$Df = 0 \tag{A}$$

where, for example, $f = \phi(x)$ and $D = \Box + m^2$ gives the free Klein-Gordon (K.G.) equation or $f = \psi(x)$, a four-component spinor, with $D = i\gamma^\mu \partial/\partial x^\mu - m$ gives the free Dirac equation.

Let $\{f\}$ denote the linear set of elements under consideration, e.g., the set of all twice differentiable functions of x for the K.G. equation, the set of all 4-component spinor functions for the Dirac equation, etc. If D denotes a (possibly nonlinear) mapping of $\{f\}$ into itself, Eq. (A) defines a subset of $\{f\}$ which we denote by $\{f\}_D$.

Let U denote a one-to-one mapping of $\{f\}$ *onto* itself. Equation (A) is said to be invariant under U if $\{f\}_D$ is invariant under U, or more directly put, if Uf is a solution whenever f is a solution:

$$Df = 0 \Rightarrow DUf = 0.$$

A sufficient condition that (A) be invariant under U is evidently that $DU = UD$ or if U^{-1} exists, as assumed, that

$$U^{-1} DU = D. \tag{I}$$

If there is a set of transformations U which leave (A) invariant, and if these transformations form a group, then (A) is said to be invariant under the group. [If (I) is satisfied for each element V of a set $\{V\}$ of one-to-one mappings, this set may be extended to a group by adjoining the identity, the inverse of any element and the product of any two elements to the set. Each element of the resulting set then satisfies (I).]

Part of the purpose of this note is (i) to exhibit a more general sufficient condition for the invariance of an equation of type (A) under a group G, (ii) to show that this more general condition is realized nontrivially by an important equation in the theory of relativistic wave equations, the square-root K.G. equation,[1] and (iii) to provide thereby a new proof of the Lorentz invariance of the square-root equation, which enables a unification to be made in the treatment of the square-root K.G. and the other relativistic wave equations. Previously, the proof of the invariance of the square-root equation has been rather special, involving the use of Fourier analysis followed by an appeal to the invariance of $\theta(p)$ under proper Lorentz transformations. These topics are treated in Secs. 2 and 3.

In Secs. 4 and 5 we extend these considerations to the case in which an external field is present. In particular, we show explicitly that the square-root equation modified in the usual way for the presence of an external electromagnetic field does *not* admit the proper Lorentz group, with $\varphi(x)$ a scalar. This fact (rather surprising, since in the classical case the equations of motion obtained from the corresponding classical Hamiltonian are of course Lorentz invariant) does not seem to be generally known. It is consistent, however, with a statement made by Dirac in motivating the linearization of the square-root equation. In discussing the (free) square-root equation, Dirac states, "... although it takes into account the relation between energy and momentum required by relativity, [it] is yet unsatisfactory from the point of view of relativistic theory, because it is very unsymmetrical between p_0

* Supported in part by the U. S. Air Force.

[1] For a discussion of the square-root equation see, e.g., S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson & Co., Evanston, Illinois), pp. 56, 64.

and the other p's, *so much so that one cannot generalize it in a relativistic way to the case when there is a field present.* We must therefore look for a new wave equation."[2]

In Sec. 6 it is shown that if the freedom allowed by gauge invariance is taken into account, the modified square-root equation is still noninvariant.

A more precise version of Dirac's general statement is formulated and discussed in Sec. 7. It would seem that a theorem of this kind is of importance in justifying statements such as "a relativistic theory of a single particle is impossible," etc. It is a basic reason for abandoning the square-root equation and facing the problem of negative energies. This point seems to have been insufficiently stressed in the literature.

2. GENERAL INVARIANCE CONDITION AND COMMUTATOR CONDITION

The requirement that U leave (A) invariant may be written in the form

$$(U^{-1}\,DU)f = 0.$$

Now since $Df = 0$, the condition (I) is certainly sufficient, but it is by no means necessary. A much more general sufficient condition for the invariance of (A) under U is that there exists an operator h such that

$$U^{-1}\,DU = h\,D, \qquad \text{(I')}$$

with the requirement that h is nonsingular on the set $\{f\}_D$. The real point is that it is sufficient (and also necessary) that $U^{-1}\,DU$ annihilate the subset $\{f\}_D$. It is not necessary that $U^{-1}\,DU$ be identical with D, which annihilates $\{f\}_D$ by definition.

Consider now the case of invariance under an n-parameter continuous group G which may be generated from a set of infinitesimal operators P_i $(i = 1, 2, \cdots n)$. We also assume now that, together with the P_i, D is a linear mapping of $\{f\}$ into itself.

In order for (I) to hold it is then both necessary and sufficient, that

$$[P_i, D] = 0, \qquad i = 1, 2, \cdots n. \qquad \text{(C)}$$

But since, as we have seen, (I) is *not* necessary for invariance, (C) is, in general, not necessary either. A more general sufficient condition than (C) is that

$$[P_i, D] = k_i\,D, \qquad i = 1, 2, \cdots n. \qquad \text{(C')}$$

where k_i is some operator nonsingular on $\{f\}_D$.

[2] P. A. M. Dirac, *Quantum Mechanics* (Oxford University Press, New York, 1947), 3rd ed., p. 254. The italics are the author's.

It can readily be shown that (C') is sufficient for (I') to hold. It is sufficient to consider the case of a 1-parameter group with $U = \exp(-aP)$. Then

$$U^{-1}\,DU = D + \sum_{n=1}^{\infty} \frac{a^n}{n!} G_n,$$

where

$$G_{n+1} = [P, G_{n-1}], \qquad G_1 = [P, D].$$

If $G_1 = h_1\,D$, it follows that if $G_n = h_n\,D$ that

$$G_{n+1} = [P, h_n\,D] = h_n[P, D] + [P, h_n]\,D = h_{n+1}\,D,$$

where

$$h_{n+1} = h_n h_1 + [P, h_n].$$

Hence (I) is satisfied with

$$h = 1 + \sum_{n=1}^{\infty} \frac{a^n}{n!} h_n.$$

Another way of describing the relation between (C) and (C') is to note that (C') ensures that the commutators with D of the infinitesimal operators of the group G annihilate the subset $\{f\}_D$, whereas (C) asserts that these commutators are identically zero. As we have seen, this is not at all necessary. We have here the counterpart of the relation between (I) and (I').

3. APPLICATION TO THE SQUARE-ROOT EQUATION

We now show that the square-root Klein-Gordon equation provides a nontrivial example of the conditions (I') and, correspondingly, (C'). By nontrivial we mean that $h \neq 1$, correspondingly, $k_i \neq 0$.

Let $\mathfrak{L}$ denote the proper homogeneous Lorentz group and let Λ denote a proper Lorentz matrix, corresponding to the Lorentz transformation

$$x' = \Lambda x. \qquad (3.1)$$

Let G denote the group of substitutions with elements $\mathfrak{S}_\Lambda$, realized on the manifold of all complex valued functions of x, via

$$\mathfrak{S}_\Lambda f(x) = f(\Lambda^{-1}x). \qquad (3.2)$$

G is then isomorphic with $\mathfrak{L}$.

That the ordinary K.G. equation,

$$(\Box + m^2)\phi(x) = 0, \qquad (3.3)$$

is invariant under G is evident by inspection, since $\Box$ is an *invariant* scalar operator: $(\partial/\partial x^\mu)(\partial/\partial x_\mu) = (\partial/\partial x'^\mu)(\partial/\partial x'_\mu)$. Equivalently,

$$\mathfrak{S}_\Lambda^{-1}\,\Box\,\mathfrak{S}_\Lambda = \Box, \qquad (3.4)$$

so that (I) is satisfied, with $D = K_x \equiv \Box + m^2$ and $U = \mathcal{S}_\Lambda$, for all Λ. The infinitesimal operators of the realization G of $\mathfrak{L}$ are given by

$$M_{\mu\nu} = x_\mu \partial/\partial x^\nu - x_\nu \partial/\partial x^\mu. \tag{3.5}$$

The condition (3.4) is then equivalent to

$$[M_{\mu\nu}, \Box] = 0, \tag{3.6}$$

so that (C) is satisfied with $D = K_x$.

The operator K_x may be written in the form

$$K_x = -K_x^{(-)} K_x^{(+)}, \tag{3.7}$$

where

$$K_x^{(\pm)} = i\,\partial/\partial x^0 \mp (-\nabla^2 + m^2)^{1/2}. \tag{3.8}$$

The equation

$$K_x^{(+)}\varphi(x) = 0 \tag{3.9}$$

is called the square-root Klein-Gordon equation. It is easy to see that

$$\mathcal{S}_\Lambda^{-1} K_x^{(+)} \mathcal{S}_\Lambda \neq K_x^{(+)}. \tag{3.10}$$

Nevertheless, Eq. (3.9) admits the group G, as is well known. The usual proof is to write $\varphi(x)$ as a Fourier integral

$$\varphi(x) = \int \tilde{\varphi}(p) e^{-ip\cdot x}\, d^4p,$$

with $\tilde{\varphi}(p) = \theta(p)\,\delta(p^2 - m^2)\phi(p)$, and $\phi(p)$ arbitrary. The restriction on $\tilde{\varphi}$ expresses the fact that the general solution of Eq. (3.9) is a superposition of plane waves of positive frequency; $p^0 = +(\mathbf{p}^2 + m^2)^{1/2}$. Now if $\varphi'(x) = \varphi(\Lambda^{-1}x)$, it follows that $\tilde{\varphi}'(p)$ is of the same form as $\tilde{\varphi}(p)$ with $\phi(p)$ replaced by $\phi'(p) = \phi(\Lambda^{-1}p)$, the crucial point being that $\theta(p) = \theta(\Lambda p)$ for a proper Lorentz transformation. Hence $\varphi'(x)$ is a solution if $\varphi(x)$ is and Eq. (3.9) admits the group G, with $\varphi(x)$ a scalar. Alternatively, one may state the results in terms of the solutions of Eq. (3.3): the separation into positive and negative frequency parts of any solution is a (proper) Lorentz covariant procedure.

We now prove that Eq. (3.9) admits G with $\varphi(x)$ a scalar, using the considerations described in section 2. In particular, we shall show that condition (C′) and hence (I′) holds.

Consider the commutators $N_{\mu\nu}$,

$$N_{\mu\nu} = [M_{\mu\nu}, K_x^{(+)}]. \tag{3.11}$$

We have

$$N_{10} = \left[-x^1 \frac{\partial}{\partial x^0} - x^0 \frac{\partial}{\partial x^1}\,,\, i\frac{\partial}{\partial x^0} - H_0 \right]$$

or

$$N_{10} = [x^1, H_0]\,\partial/\partial x^0 - \left[x^0, i\frac{\partial}{\partial x^0}\right]\frac{\partial}{\partial x^1}. \tag{3.12}$$

Here we have introduced the abbreviation

$$H_0 = (-\nabla^2 + m^2)^{1/2}.$$

The first commutator in Eq. (3.12) may be computed most simply by recalling that if

$$[q, p] = 1,$$

then not only

$$[g(q), p] = g'(q),$$

but also

$$[l(p), q] = -l'(p).$$

Putting $x^1 = q$, $\partial/\partial x^1 = p$ and $H_0 = l(p)$ where

$$l(p) = (-p^2 - \partial^2/\partial x_2^2 - \partial^2/\partial x_3^2 + m^2)^{1/2},$$

we have

$$[q, l(p)] = l'(p) = -p/l(p).$$

Thus,

$$N_{10} = -(\partial/\partial x^1)H_0^{-1}\,\partial/\partial x^0 - i\,\partial/\partial x^1$$

so that, recalling Eq. (3.8) we get:

$$N_{i0} = i(\partial/\partial x^i)H_0^{-1}K_x^{(+)}, \qquad (j = 1, 2, 3). \tag{3.13}$$

The remaining $N_{\mu\nu}$ ($\mu \neq 0$, $\nu \neq 0$) vanish, corresponding to the invariance of $K_x^{(+)}$ under ordinary rotations. We see from Eq. (3.13) that N_{i0} indeed is $\neq 0$, so that (C) is violated but (C′) is satisfied.

The Lorentz invariance of Eq. (3.8) is thereby proved and at the same time an example of (C′) is obtained. It is clear that, since (C′) includes (C), the use of (C′) allows the question of the invariance of the usual relativistic wave equations, including the square-root equation, to be handled in an uniform way, without going to momentum space.

4. MODIFICATION FOR EXTERNAL FIELDS

Most of the "free" relativistic wave equations have the form of Eq. (A) with f a column vector $\chi(x)$ and D a matrix with elements which are functions of the differential operators $\partial/\partial x^\mu$. We thus write, more explicitly:

$$D[\partial/\partial x^\mu]\chi(x) = 0 \tag{4.1}$$

Interaction with an external, local, tensor field of rank n, $T^{(n)}(x)$ is included by introducing a dependence of the elements of D on the components

$T^{\mu_1,\mu_2,\cdots,\mu_n}(x)$ of $T^{(n)}$ as well. Thus we write, instead of Eq. (4.1),

$$D[\partial/\partial x^\mu; T^{(n)}(x)]\chi(x) = 0. \tag{4.2}$$

For simplicity, consider the case in which χ has one component only. Equation (4.2) is said to admit $\mathcal{L}$, with χ a scalar, if it follows from it that also

$$D[\partial/\partial x^\mu; T'^{(n)}(x)]\chi'(x) = 0 \tag{4.3}$$

with

$$\chi'(x) = \chi(\Lambda^{-1}x) \tag{4.4a}$$

and

$$T'^{(n)}(x) = S_\Lambda T^{(n)}(\Lambda^{-1}x), \tag{4.4b}$$

where

$$S_\Lambda T^{\mu_1\cdots\mu_n} = \Lambda^{\mu_1}_{\nu_1}\cdots\Lambda^{\mu_n}_{\nu_n}T^{\nu_1\cdots\nu_n}, \tag{4.4c}$$

whatever Λ.

The analog of the set $\{f\}$ of Sec. 1 is here the set $\{F\}$ of all ordered pairs of elements of the form $F = [\chi(x); T^{(n)}(x)]$. The analog of $\{f\}_D$ is the subset, $\{F\}_D$ of all pairs F satisfying Eq. (4.2). The group $\mathcal{G}$ under which Eq. (4.2) is invariant is the direct product of the realizations of $\mathcal{L}$ effected by the $\chi(x)$ and the $T^{(n)}(x)$ separately. Thus $\mathcal{G} = \{\mathcal{G}_\Lambda\}$, where $\mathcal{G}_\Lambda F = [\chi'(x); T'^{(n)}(x)]$. For fixed $T^{(n)}$, D is, in cases of interest, a linear operator but $\{F\}_D$ is clearly not a linear space in general.

Since $\chi'(x) = \mathcal{S}_\Lambda\chi(x)$, we see, on multiplying Eq. (4.3) by $\mathcal{S}_\Lambda^{-1}$, that the analog of (I') is here the condition

$$\mathcal{S}_\Lambda^{-1}\, D[\partial/\partial x^\mu; S_\Lambda T^{(n)}(\Lambda^{-1}x)]\mathcal{S}_\Lambda = h\, D[\partial/\partial x^\mu; T^{(n)}(x)], \tag{E'}$$

with h nonsingular on the domain annihilated by D, with $T^{(n)}$ fixed. A more convenient form of (E') is obtained by taking the operators $\mathcal{S}_\Lambda$, $\mathcal{S}_\Lambda^{-1}$ "inside" D, so that, using

$$\mathcal{S}_\Lambda^{-1}(\partial/\partial x^\mu)\mathcal{S}_\Lambda = \Lambda^\mu_\nu(\partial/\partial x^\nu), \tag{4.5}$$

and

$$\mathcal{S}_\Lambda^{-1}T^{(n)}(\Lambda^{-1}x)\mathcal{S}_\Lambda = T^{(n)}(x), \tag{4.6}$$

we get

$$D[\Lambda^\nu_\mu(\partial/\partial x^\nu); S_\Lambda T^{(n)}(x)] = h\, D[\partial/\partial x^\mu; T^{(n)}(x)]. \tag{$\bar{\text{E}}$}$$

The analog of (I) is the more stringent condition (E) obtained from either (E') or ($\bar{\text{E}}$) by putting $h = 1$, i.e.,

$$D[\Lambda^\nu_\mu(\partial/\partial x^\nu); S_\Lambda T^{(n)}(x)] = D[\partial/\partial x^\mu; T^{(n)}(x)]. \tag{E}$$

Condition (E) will be satisfied if and only if D is constructed as a scalar in terms of the vector $\partial/\partial x^\mu$ and the tensor field $T^{(n)}$.

A well-known example of (E) results from the K.G. equation for a particle of charge e in an external electromagnetic field $A^\mu(x)$, in which case

$$D = D[\partial/\partial x^\mu; A^\nu(x)] = \pi_\mu\pi^\mu + m^2, \tag{4.7}$$

where

$$\pi_\mu = \partial/\partial x^\mu + ieA_\mu. \tag{4.8}$$

(D is obtained from the operator $K_x = \Box + m^2$ by letting $\partial/\partial x^\mu \to \pi_\mu$). The external field K.G. equation therefore admits $\mathcal{L}$, with $\chi(x)$ a scalar.

Consider, however, the corresponding modification of the square-root K.G. equation:

$$\{i\,\partial/\partial x^0 - eA_0 - [(-i\nabla - e\mathbf{A})^2 + m^2]^{1/2}\} \times \varphi(x) = 0, \tag{4.9}$$

or, if we write

$$K_x^{(+)} = K_x^{(+)}[\partial/\partial x^\mu] = i\,\partial/\partial x^0 - [(i\,\partial/\partial x^i)^2 + m^2]^{1/2}, \tag{4.10}$$

equivalently but more succinctly,

$$K_x^{(+)}[\pi_\mu]\varphi(x) = 0. \tag{4.11}$$

We prove in the next section that Eq. (4.11) does not admit $\mathcal{L}$, with φ a scalar. Clearly, in this case $D = K_x^{(+)}[\pi_\mu]$ is not a scalar. But the free field case, considered in the preceding section, has shown that the scalar nature of D is only a sufficient condition: $K_x^{(+)}[\partial/\partial x^\mu]$ is also not a scalar, nevertheless, with $e = 0$, Eq. (4.11) admits the group $\mathcal{L}$. A proof is therefore necessary to show that, in particular, the more general condition ($\bar{\text{E}}$) or (E') does not hold, if $e \neq 0$.

5. NONINVARIANCE OF THE MODIFIED SQUARE-ROOT EQUATION

We shall show that there exist electromagnetic fields A^μ and solutions of Eq. (4.11) that do not also satisfy

$$K_x^{(+)}[\Lambda^\nu_\mu\pi_\nu]\varphi(x) = 0. \tag{5.1}$$

As a tool, we shall need the answer to the following problem: Let A and B denote noncommuting linear operators, with A positive definite. Let λ be a real parameter and let

$$Q = Q(\lambda) = A + \lambda B. \tag{5.2}$$

We ask: What is $(Q)^{1/2}$, correct to terms of order λ?

We note that

$$Q^{-1/2} = \pi^{-1/2} \int_0^\infty e^{-Qu} u^{1/2}\, du, \tag{5.3}$$

so that, on integration with respect to Q, from 0 to Q, we get

$$Q^{1/2} = (\pi^{-1/2}/2) \int_0^\infty (1 - e^{-Qu}) u^{-3/2}\, du. \tag{5.4}$$

Feynman's operator calculus[3] can now be used to expand e^{-Qu} in a power series in λ:

$$e^{-(A+\lambda B)u} = e^{-Au} - \lambda u \int_0^1 e^{-Aus} B e^{-Au(1-s)}\, ds + \cdots . \tag{5.5}$$

It follows that[4]

$$Q^{1/2} = A^{1/2} + \tfrac{1}{2}\lambda \Gamma_A[B] + O(\lambda^2) \tag{5.6}$$

where

$$\Gamma_A[B] = \pi^{-1/2} \int_0^\infty du u^{-1/2} \int_0^1 ds e^{-Aus} B e^{-Au(1-s)}. \tag{5.7}$$

As a check, note that if $[B, A] = 0$, a simple integration gives

$$\Gamma_A[B] \to \Gamma_A[1]B = A^{-1/2}B, \tag{5.8}$$

so that $Q^{1/2} \to A^{1/2}(1 + \lambda B/2A + \cdots)$ as required.

Returning to Eq. (5.1), we consider a Lorentz transformation in the direction of the x^1 axis, with velocity β. Equation (5.1) then assumes the form

$$K(\beta)\varphi(x) = 0, \tag{5.9}$$

where

$$K(\beta) = i(\gamma\pi_0 - \beta\gamma\pi_1) - [-(\beta\gamma\pi_0 + \gamma\pi_1)^2 - \pi_2^2 - \pi_3^2 + m^2]^{1/2}, \tag{5.10}$$

with $\gamma = (1 - \beta^2)^{-1/2}$, and Eq. (4.9) is simply

$$K(0)\varphi(x) = 0. \tag{5.11}$$

We now expand

$$K(\beta) = K(0) + \beta K'(0) + (\beta^2/2)K''(0) + \cdots ,$$

so that Eq. (5.9) implies,

$$K'(0)\varphi(x) = 0. \tag{5.12}$$

Clearly $K'(0) \neq 0$, but it is necessary to show more, for $K'(0)$ need only annihilate $\{\varphi\}_0$, the subspace of solutions of Eq. (5.11) for fixed A^μ. To compute $K'(0)$ we need the quantity under the square root in Eq. (5.10) only to terms of order β. It is also sufficient to restrict our attention to fields which in the (arbitrary) frame under consideration are purely electrostatic, i.e., have $\mathbf{A} = 0$ and A_0 independent of x^0. With these simplifications in mind, we set

$$A = -\nabla^2 + m^2 \tag{5.13}$$

$$B = [\pi_0, \partial/\partial x^1]_+ \tag{5.14}$$

and use Eq. (5.6), with $\beta = \lambda$, to expand the square root. Thus we get

$$K(\beta) = i(\pi_0 - \beta\, \partial/\partial x^1) - A^{1/2} - (\beta/2)\Gamma_A[B] + O(\beta^2), \tag{5.15}$$

so that

$$K'(0) = -i\, \partial/\partial x^1 - \tfrac{1}{2}\Gamma_A[B], \tag{5.16}$$

with

$$K(0) = i\pi_0 - (-\nabla^2 + m^2)^{1/2}. \tag{5.17}$$

To produce an explicit counter example, showing that $K'(0)$ does not annihilate the solutions of

$$[i\pi_0 - (-\nabla^2 + m^2)^{1/2}]\varphi(x) = 0, \tag{5.18}$$

we assume that A_0 is independent of x^1 also, so that

$$B \to 2\frac{\partial}{\partial x^0}\frac{\partial}{\partial x^1} + 2ieA_0\frac{\partial}{\partial x^1}. \tag{5.19}$$

Since $\Gamma_A(1) = A^{-1/2}$, we get:

$$K'(0) = -i\frac{\partial}{\partial x^1} - A^{-1/2}\frac{\partial}{\partial x^0}\frac{\partial}{\partial x^1} - ie\Gamma_A[A_0]\frac{\partial}{\partial x^1},$$

or

$$K'(0) = i\frac{\partial}{\partial x^1}\left[A^{-1/2}\left(i\frac{\partial}{\partial x^0} - A^{1/2}\right) - e\Gamma_A[A_0]\right]. \tag{5.20}$$

Hence, on use of Eq. (5.18), Eq. (5.12) reduces, if $e \neq 0$, to

$$(A^{-1/2}A_0 - \Gamma_A[A_0])\, \partial\varphi/\partial x^1 = 0. \tag{5.21}$$

Now consider a solution of Eq. (5.18) that is expandable in a power series in e:

$$\varphi = \sum_{n=0}^\infty e^n \varphi_n, \tag{5.22}$$

so that

$$K_x^{(+)}\varphi_0 = 0 \tag{5.23}$$

and

$$K_x^{(+)}\varphi_n = A_0\varphi_{n-1}, \qquad n \geq 1. \tag{5.24}$$

Then Eq. (5.21) implies that

$$(A^{-1/2}A_0 - \Gamma_A[A_0])\, \partial\varphi_0/\partial x^1 = 0. \tag{5.25}$$

[3] R. P. Feynman, Phys. Rev. **108**, 84 (1951).

[4] This result is also contained in J. Sucher, Ph.D. Thesis Columbia University, 1958 (unpublished).

Since $\varphi_0(x)$ at, say, $x^0 = 0$, is essentially arbitrary, so is $\partial\varphi_0/\partial x^1$ at $x^0 = 0$, and hence, Eq. (5.25) is in general not satisfied.

To be completely explicit, we may take[5]

$$\varphi_0(x) = e^{-ik\cdot x}, \qquad A_0(x) = e^{i\mathbf{q}\cdot\mathbf{x}},$$

with $k^1 \neq 0$, but $q^1 = 0$. Then

$$\Gamma_A[A_0]\varphi_0 \to \int_0^\infty du\, u^{-1/2} \int_0^1 ds e^{-aus} e^{-bu(1-s)} A_0\varphi_0$$
$$= [2/(a^{1/2} + b^{1/2})]A_0\varphi_0,$$

where

$$a = (\mathbf{q} + \mathbf{k})^2 + m^2, \qquad b = \mathbf{k}^2 + m^2,$$

and

$$A^{-1/2}A_0\varphi_0 \to a^{-1/2}A_0\varphi_0.$$

Hence, unless $\mathbf{q} = 0$, Eq. (5.25) is not satisfied since it requires $(a)^{1/2} + (b)^{1/2} = 2(a)^{1/2}$.

6. NON INVARIANCE WITH ARBITRARY PHASE TRANSFORMATION

The proof of the fact that Eq. (4.11) does not admit $\mathfrak{L}$, with φ a scalar, was really carried out for an arbitrary external vector field. For the case of an electromagnetic field, there is the freedom of gauge transformations:

$$\left.\begin{aligned} A_\mu &\to A_\mu + \partial\Phi/\partial x^\mu, \\ \varphi(x) &\to e^{-ie\Phi}\varphi(x), \end{aligned}\right\} \tag{6.1}$$

and, indeed, both the external field K.G. equation and the external field square-root equation admit this gauge group.

In a given frame, starting from a pair $\{\varphi; A^\mu\}$, the set obtainable from these by gauge transformations forms an equivalence class, all elements describing the same state. In the case of the external K.G. equation, the Lorentz invariance is such that elements of the equivalence class directly transform to *corresponding* elements of the equivalence class describing the same state in a different frame. By *corresponding* we mean that $A^\mu \to \Lambda^\mu_\nu A^\nu$ without an additional gauge transformation. The K.G. equation is invariant not only under (6.1) and under

$$\left.\begin{aligned} \varphi \to \varphi'(x) &= \varphi(\Lambda^{-1}x), \\ A_\mu \to A'_\mu(x) &= \Lambda^\nu_\mu A_\nu(\Lambda^{-1}x), \end{aligned}\right\} \tag{6.2}$$

but therefore under *combined* Lorentz and gauge transformations performed successively and independently.

Off hand, it might seem possible to construct an equation relating a (scalar) wavefunction $\varphi(x)$ and an electromagnetic field $A^\mu(x)$ in such a way that the equation admitted not Eq. (6.2), but instead the substitution

$$\left.\begin{aligned} \varphi \to \varphi'(x) &= \varphi(\Lambda^{-1}x), \\ A_\mu \to A'_\mu(x) &= \Lambda^\nu_\mu A_\nu(\Lambda^{-1}x) + \partial\bar{\Gamma}/\partial x^\mu, \end{aligned}\right\} \tag{6.3}$$

for some suitable choice of $\bar{\Gamma} = \bar{\Gamma}(x)$. Such an equation would also be said to admit $\mathfrak{L}$ since it would still provide a Lorentz-invariant manifold of states (equivalence classes); there does not seem to be a physical reason for requiring that the individual elements of Lorentz equivalent classes map onto each other according to Eq. (6.2). Equation (6.3) corresponds only to a reshuffling (in the transformed reference frame) of the pairing of the wave functions φ' and the four-potential A'_μ used to represent the field $F'_{\mu\nu}$. $\Gamma(x)$ may vary not only with the Lorentz transformation but may also depend on the pair $[\varphi; A^\mu]$.

We can show, however, that Eq. (4.11) is not invariant in this extended sense either. For this purpose it is convenient to use the fact that Eq. (4.11) is invariant under gauge transformations.

Substituting, according to Eq. (6.3), into Eq. (4.11) we obtain

$$K^{(+)}_x[\partial/\partial x^\mu + ieA'_\mu(x) + ie\,\partial\bar{\Gamma}/\partial x^\mu]S_\Lambda\varphi(x) = 0.$$

Multiplying by S^{-1}_Λ on the left we obtain, using Eqs. (4.6) and (4.7) we get

$$K^{(+)}_x[\Lambda^\nu_\mu(\pi_\nu + \partial\Gamma(x)/\partial x^\nu)]\varphi(x) = 0, \tag{6.4}$$

where

$$\Gamma(x) = \bar{\Gamma}(\Lambda^{-1}x), \tag{6.5}$$

so that, corresponding to the gauge invariance of (4.11), we get

$$K^{(+)}_x[\Lambda^\nu_\mu\pi_\nu]e^{-ie\Gamma(x)}\varphi(x) = 0. \tag{6.6}$$

To prove the noninvariance in the extended sense under consideration, it is again sufficient to consider Lorentz transformation in the direction of the x^1 axis. We exhibit the dependence of Γ on the velocity β explicitly by writing $\Gamma(x;\beta)$ for $\Gamma(x)$, and so write Eq. (6.6) in the form

$$K(\beta)e^{-ie\Gamma(x;\beta)}\varphi(x) = 0. \tag{6.7}$$

Since for $\beta = 0$ we must have $\Gamma(x;0) = 1$, we get, on expanding the following left-hand side in a power series in β:

$$[K(0) + K'(0)\beta + \cdots]$$
$$\times [1 - ie\Gamma^{(1)}(x)\beta + \cdots]\varphi(x) = 0,$$

[5] We should really take $A_0(x) = \mathrm{Re}\exp[i\mathbf{q}\cdot\mathbf{x}]$, but it is easy to see that the same conclusion would be reached.

where

$$\Gamma^{(1)}(x) = (\partial/\partial\beta)\Gamma(x;\beta)\,|_{\beta=0},$$

so that we require

$$[-ieK(0)\Gamma^{(1)}(x) + K'(0)]\varphi(x) = 0. \quad (6.8)$$

If $\Gamma^{(1)} \neq 0$, this may be solved for $\Gamma^{(1)}$:

$$\Gamma^{(1)}(x) = -(i/e)K^{-1}(0)K'(0)\varphi(x), \quad (6.9)$$

where $K^{-1}(0)$ is a Green's function for $K(0)$. In fact, the higher derivatives of $\Gamma(x;\beta)$ at $\beta = 0$ may be found in a similar way, so that formally, at least, one may construct a Γ (which is a function of x and β and a functional of φ and A^μ) such that Eq. (6.6) is satisfied. However, for the case of the electromagnetic field A^μ, the function $\Gamma(x;\beta)$ must be *real*, so that $\Gamma^{(1)}(x)$ must also be real. But clearly the right-hand side of Eq. (6.9) is like K^{-1}, K', and $\varphi(x)$, in general complex so that a contradiction is obtained if $\Gamma^{(1)} \neq 0$. [This may be made explicit, as in the previous section, by expanding the r.h.s. of Eq. (6.9) in powers of e, with the choices for A^μ and φ_0 as before.] Hence, $\Gamma^{(1)} = 0$ and Eq. (6.8) reduces to Eq. (5.12) of the preceding section, $K'(0)\varphi = 0$, which, as has been seen, is in general not a consequence of Eq. (4.11).

7. DISCUSSION

We have seen that the square-root K.G. equation modified for the presence of an external electromagnetic field in the usual way, does not admit the Lorentz group, with the wave function a scalar, even allowing for the extra freedom permitted by gauge invariance.

Another equation considered occasionally is the square-root analog of the K.G. equation in the presence of an external scalar field $U(x)$:

$$[\Box + m^2 + \lambda U(x)]\varphi(x) = 0, \quad (7.1)$$

and correspondingly

$$\{i\,\partial/\partial x^0 - [-\nabla^2 + m^2 + \lambda U(x)]^{1/2}\}\varphi(x) = 0. \quad (7.2)$$

Although (7.1) admits $\mathfrak{L}$, with $\varphi(x) \to \varphi(\Lambda^{-1}x)$, $U(x) \to U(\Lambda^{-1}x)$, it may be shown by using the methods of Sec. 5, that Eq. (7.2) does not.

Both Eq. (4.11) and (7.2) may be written in the form

$$\{K_x^{(+)}[\partial/\partial x^\mu] - I[\partial/\partial x^\mu; \lambda T^{(n)}(x)]\}\varphi(x) = 0, \quad (7.3)$$

where the interaction operator I, assumed to be defined for λ in some neighborhood of 0, vanishes as $\lambda \to 0$. Dirac's statement then corresponds to the assertion that for no choice of $I \neq 0$, such that $I \to 0$ for $\lambda \to 0$, does Eq. (7.3) admit $\mathfrak{L}$. The mathematical problem is then to show that for no choice of I does Eq. (7.3) imply also that

$$\{K_x^{(+)}[\Lambda_\mu^\nu(\partial/\partial x^\nu)] - I[(\Lambda_\mu^\nu\,\partial/\partial x^\nu); \lambda S_\Lambda T^{(n)}(x)]\}\varphi(x) = 0. \quad (7.4)$$

It seems likely that the methods used in Secs. 5 and 6 would be useful in the study of this problem.[6]

Note that although the interaction operators considered are nonlocal, the interaction is with a *local* field in the sense that I is required to be a functional of a local field. The problem may be generalized to include interactions which are functionals of nonlocal tensor fields. It would be quite interesting to settle the question in this more general context also.[7] In either case, it would be amusing to know whether or not a conserved current can be constructed, bilinear in φ as for the free square-root equation.

In conclusion, we note that several authors[8] have shown, at least the formal possibility of the existence of a relativistic theory of two particles in interaction within a Hamiltonian framework. More recently, an explicit example of such a theory, untroubled by convergence questions, has been obtained.[9] The connection between the limits of such a theory as one of the masses becomes infinite, and the problem posed in this section would seem to merit further study.

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[6] These methods have in fact been used to obtain a proof of the noninvariance of Eq. (7.4) for some simple classes of interactions I.

[7] Another possibility is a nonlocal transformation law for $\varphi(x)$. The interpretation problem for such equations would have to be faced in any case.

[8] B. Bakamjian and L. H. Thomas, Phys. Rev. **92**, 1300 (1953); L. L. Foldy, *ibid.* **122**, 275, 1961; E. C. G. Sudarshan (unpublished).

[9] E. C. G. Sudarshan (private communication).

Normalization Condition for the Bethe-Salpeter Wavefunction and a Formal Solution to the Bethe-Salpeter Equation*

IWAO SATO†
Department of Physics, University of Maryland, College Park, Maryland
(Received 23 July 1962)

By the use of an inhomogeneous Bethe-Salpeter equation, a normalization condition for the Bethe-Salpeter wavefunction is obtained. This condition requires the normalization integral to be positive. A formal solution is obtained in the ladder approximation, and convergence of the normalization integral is proved by the use of this solution. This solution is also used to prove a dispersion relation for the vertex function of the compound particle and to give an approximate solution The positiveness of the normalization integral is proved in the nonrelativistic limit. The bound state of nucleon and antinucleon is studied in the ladder-chain approximation and it is found that the normalization condition gives a finite wavefunction in spite of divergency of the normalization integral.

INTRODUCTION

A DISPERSION-theoretic approach to the bound-state problem in quantum field theory has been proposed by Blankenbecler and Cook.[1] However, they merely assumed the basic dispersion relation without proof. Also, they have not given any prescription to calculate the magnitude of the "wavefunction," which is required for the calculation of some observables related to the bound states. In view of these facts, we think it still worthwhile to study another approach which is based on the Bethe-Salpeter equation.

In the present paper we confine ourselves to the case in which all the elementary particles are spinless. In Sec. 1 we introduce something like a field operator of the compound particle and start with an inhomogeneous Bethe-Salpeter equation. Then the bound-state solutions are classified as the scalar solution, vector solution, and so on, according to the transformation property of that field operator. In virtue of the use of the inhomogeneous equation, we can obtain a condition to fix the magnitude of the Bethe-Salpeter wavefunction. We refer to this condition as the normalization condition. We find that this condition requires a certain integral which we refer to as the normalization integral to be positive. In order to examine the normalizability in more detail, we try to solve the Bethe-Salpeter equation in the ladder approximation and obtain a formal scalar solution in Sec. 2. Using this solution, we prove convergence of the normalization integral and also give an approximation method based on this solution. This solution is also used in Sec. 3 to prove that the dispersion relation assumed by Blankenbecler and Cook really holds in the ladder approximation. As a preparation for extending our method to the case of practical interest, we study the vector solution in Sec. 4. The normalization integral is again found to be convergent, though at first sight it looks divergent. Also, it is found that the abnormal S-state solution, which is an odd function of the relative time, appears as the longitudinal vector solution. Unfortunately, we cannot draw any conclusion about the sign of the normalization integral in the relativistic cases. We therefore study the nonrelativistic limit of our equations in Sec. 5 and find that the normalization integrals are always positive in this limit. As an example of the case where the divergence appears, in Sec. 6 we study the bound state of nucleon and antinucleon in the ladder-chain approximation of Okubo and Feldman.[2] We find that the Bethe-Salpeter wavefunction remains finite, though the normalization integral is divergent. We also find that the positiveness of the normalization integral corresponds to the requirement $Z_3 > 0$ in the renormalization theory.

1. NORMALIZATION CONDITION FOR THE BETHE-SALPETER WAVE FUNCTION

We suppose that two scalar fields, which we refer to as proton and neutron fields, are interacting through a neutral scalar meson field and consider the following function:

$$K(x_1, x_2; x_3, x_4) \equiv \langle 0 \,|T(\varphi_p(x_1)\varphi_n(x_2)\varphi_p^\dagger(x_3)\varphi_n^\dagger(x_4))|\, 0\rangle, \tag{1.1}$$

* Supported by the U. S. Air Force.
† On leave of absence from Tôhoku University, Sendai, Japan.
[1] R. Blankenbecler and L. F. Cook, Jr., Phys. Rev. **119**, 1745 (1960).
[2] S. Okubo and D. Feldman, Phys. Rev. **117**, 279 (1960).

where φ_p and φ_n are the Heisenberg field operators for proton and neutron and $|0\rangle$ stands for the physical vacuum. According to Salpeter and Bethe, and Gell-Mann and Low,[3] this function obeys the integral equation

$$K(x_1, x_2; x_3, x_4) = \Delta_p(x_1 - x_3)\,\Delta_n(x_2 - x_4) + \int d^4x_5 \cdots d^4x_8\, \Delta_p(x_1 - x_5)\,\Delta_n(x_2 - x_6) \times G(x_5, x_6; x_7, x_8)K(x_7, x_8; x_3, x_4), \quad (1.2)$$

where the definition of the kernel G is given in reference 3, and Δ_p and Δ_n are the Feynman propagators for proton and neutron. For simplicity, we assume equal mass m for proton and neutron, and neglect the radiative corrections to Δ_p and Δ_n.

If we make x_3 equal to x_4, the Fourier-integral representation of K has the following form:

$$K(x_1, x_2; x, x) = -(2\pi)^{-8} \int d^4q\, d^4P F(q, P) \times \exp\left[i(\tfrac{1}{2}P + q)x_1 + i(\tfrac{1}{2}P - q)x_2 - iPx\right]. \quad (1.3)$$

Inserting this into (1.2), we have

$$F(q, P) = [(\tfrac{1}{2}P + q)^2 + m^2]^{-1}[(\tfrac{1}{2}P - q)^2 + m^2]^{-1} \times \left[1 + \int d^4q' G(q, q'; P)F(q', P)\right], \quad (1.4)$$

where $G(q, q'; P)$ is the Fourier transform of $G(x_1, \cdots, x_4)$. Throughout this paper we suppress the infinitesimal negative imaginary parts in the masses.

Now let us suppose that there is a scalar composite particle of proton and neutron, which we refer to as the scalar deuteron. We denote its mass by m_d. Then, slightly extending the usual procedure, we can easily derive the equation

$$\int d^4x \exp(i\,Dx)(m_d^2 - \Box_x)K(x_1, x_2; x, x) = -i2V\,D_0\langle 0\,|T(\varphi_p(x_1)\varphi_n(x_2))|\,D\rangle\langle D\,|\varphi_p^\dagger(0)\varphi_n^\dagger(0)|\,0\rangle$$

where $|D\rangle$ is the single deuteron state with four-momentum D that satisfies $D^2 = -m_d^2$. Inserting (1.3) into the left-hand side of this equation, we have

$$\chi(x_1, x_2; D) \equiv (2V\,D_0)^{1/2}\langle 0\,|T(\varphi_p(x_1)\varphi_n(x_2))|\,D\rangle = -iN^*(2\pi)^{-4} \int d^4q f(q, D) \times \exp\left[i(\tfrac{1}{2}D + q)x_1 + i(\tfrac{1}{2}D - q)x_2\right], \quad (1.5)$$

where

$$f(q, D) = [(m_d^2 + P^2)F(q, P)]_{P=D}, \quad (1.6)$$

$$N^{-1} = (2V\,D_0)^{1/2}\langle 0\,|\varphi_p(0)\varphi_n(0)|\,D\rangle. \quad (1.7)$$

If x_1 and x_2 are set equal to zero in (1.5), the left-hand side becomes N^{-1}. Therefore, we have

$$|N|^{-2} = -i(2\pi)^{-4} \int d^4q f(q, D). \quad (1.8)$$

Since (1.4) is an inhomogeneous integral equation, its solution $F(q, P)$ is uniquely determined. Because of (1.6), $-m_d^2$ is determined as a pole of $F(q, P)$ as a function of P^2, and $f(q, D)$ is given by the residue of $F(q, P)$. Therefore, $f(q, D)$ is also uniquely determined. Then the absolute value of N is determined by means of (1.8). Inserting the result into (1.5), we can determine the absolute magnitude of the Bethe-Salpeter wavefunction χ. We therefore refer to (1.8) as the normalization condition. In order that the wavefunction may be normalizable, the right-hand side of (1.8) must be positive. However it is possible that $F(q, P)$ has poles for which the right-hand side of (1.8) is negative. The bound states corresponding to such poles will be the so-called ghost states. In fact, we show in Sec. 6 that, in a certain case, negativeness of the right-hand side of (1.8) is the condition for appearance of the ghost in the renormalization theory.

The above consideration can be easily extended to the vector deuteron case. In this case we consider the function

$$L_\mu(x_1, x_2; x) \equiv \frac{i}{2}\left[\left(\frac{\partial}{\partial x_{3\mu}} - \frac{\partial}{\partial x_{4\mu}}\right)K(x_1, x_2; x_3, x_4)\right]_{x_3 = x_4 = x}. \quad (1.9)$$

The Fourier representation of this function has the form

$$L_\mu(x_1, x_2; x) = -(2\pi)^{-8} \int d^4q\, d^4P F_\mu(q, P) \times \exp\left[i(\tfrac{1}{2}P + q)x_1 + i(\tfrac{1}{2}P - q)x_2 - iPx\right]. \quad (1.10)$$

In order to decompose F_μ into the transversal and longitudinal parts, we introduce three unit four-vectors $e_\mu^{(\alpha)}$ ($\alpha = 1, 2, 3$) which satisfy $e^{(\alpha)} \cdot e^{(\beta)} = \delta_{\alpha\beta}$ and $e^{(\alpha)} \cdot P = 0$ and write

$$F_\mu(q, P) = \sum_{\alpha=1}^{3} e_\mu^{(\alpha)}(e^{(\alpha)} \cdot q)F_t(q, P) + P_\mu F_l(q, P). \quad (1.11)$$

Then it is easily found that (1.2) gives

[3] E. E. Salpeter and H. A. Bethe, Phys. Rev. **84**, 1232 (1951); M. Gell-Mann and F. Low, *ibid.* **84**, 350 (1951).

$$(e^{(\alpha)}\cdot q)F_t(q,P) = [(\tfrac{1}{2}P+q)^2+m^2]^{-1}[(\tfrac{1}{2}P-q)^2+m^2]^{-1} \times\Big[(e^{(\alpha)}\cdot q)+\int d^4q'G(q,q';P) \times(e^{(\alpha)}\cdot q')F_t(q',P)\Big], \tag{1.12}$$

$$F_t(q,P) = [(\tfrac{1}{2}P+q)^2+m^2]^{-1}[(\tfrac{1}{2}P-q)^2+m^2]^{-1} \times\Big[(P\cdot q)/P^2+\int d^4q'G(q,q';P)F_t(q',P)\Big]. \tag{1.13}$$

In (1.12), the factor $(e^{(\alpha)}\cdot q)$ appears also in the integral after carrying out the integration, so we can finally drop this factor from the both sides. This justifies that F_μ can be written in the form (1.11).

If we assume the existence of a transversal vector deuteron with mass m_d, we have from (1.9)

$$\int d^4x\,\exp(iDx)(m_d^2-\Box_x)L_\mu(x_1,x_2;x) = -i\sum_{\alpha=1}^{3}(2V\,D_0)^{1/2} \times\langle 0\,|T(\varphi_p(x_1)\varphi_n(x_2))|\,D,e^{(\alpha)}\rangle e_\mu^{(\alpha)}/N^*, \tag{1.14}$$

where $|D,e^{(\alpha)}\rangle$ denotes the single deuteron state with four-momentum D and polarization vector $e^{(\alpha)}$, and we have put

$$e_\mu^{(\alpha)}/N = (2V\,D_0)^{1/2}\Big\langle 0\,\Big|\,\tfrac{1}{2}i\Big[\varphi_p(x)\frac{\partial\varphi_n(x)}{\partial x_\mu} - \frac{\partial\varphi_p(x)}{\partial x_\mu}\varphi_n(x)\Big]_{x=0}\Big|\,D,e^{(\alpha)}\Big\rangle. \tag{1.15}$$

Inserting (1.10) with (1.11) for F_μ into the left-hand side of (1.14), we have

$$\chi_t(x_1,x_2;D,e^{(\alpha)}) \equiv (2V\,D_0)^{1/2}\langle 0\,|T(\varphi_p(x_1)\varphi_n(x_2))|\,D,e^{(\alpha)}\rangle = -iN^*(2\pi)^{-4}\int d^4q(e^{(\alpha)}\cdot q)f_t(q,D) \times\exp[i(\tfrac{1}{2}D+q)x_1+i(\tfrac{1}{2}D-q)x_2], \tag{1.16}$$

where

$$f_t(q,D) = [(m_d^2+P^2)F_t(q,P)]_{P=D}. \tag{1.17}$$

From (1.15) and (1.16) we have the normalization condition

$$|N|^{-2} = -i(2\pi)^{-4}\int d^4q(e^{(\alpha)}\cdot q)^2 f_t(q,D). \tag{1.18}$$

The right-hand side of this equation is really independent of $e^{(\alpha)}$ because $e^{(\alpha)}$ is perpendicular to D.

In the same way, if we assume the existence of a longitudinal vector deuteron, we have the following result:

$$\chi_l(x_1,x_2;D) \equiv (2V\,D_0)^{1/2}\langle 0\,|T(\varphi_p(x_1)\varphi_n(x_2))|\,D,l\rangle = -iN^*(2\pi)^{-4}\int d^4q f_l(q,D) \times\exp[i(\tfrac{1}{2}D+q)x_1+i(\tfrac{1}{2}D-q)x_2], \tag{1.19}$$

where

$$f_l(q,D) = [(m_d^2+P^2)F_l(q,P)]_{P=D}, \tag{1.20}$$

and the absolute value of N is determined by

$$|N|^{-2} = i(2\pi)^{-4}m_d^{-2}\int d^4q(q\cdot D)f_l(q,D). \tag{1.21}$$

2. SCALAR SOLUTION IN THE LADDER APPROXIMATION

In this section we give a formal solution to the inhomogeneous Bethe-Salpeter equation (1.4) in the ladder approximation and, on its basis, we discuss the normalizability of the wavefunction and a possible approximation method. In the ladder approximation the kernel G is expressed as

$$G(q,q';P) = -i\lambda\pi^{-2}[(q-q')^2+\mu^2]^{-1}, \tag{2.1}$$

where μ is mass of the meson. Wick[4] has shown that (1.4) with (2.1) can be transformed into a non-singular Fredholm integral equation by bringing q_0 on the imaginary axis and we could obtain a formal solution using Wick's equation. We intend, however, to examine later the connection between our method and the dispersion-theoretic method by Blankenbecler and Cook. For this purpose it is convenient to express F as

$$F(q,P) = \frac{1}{2}\int_{-1}^{1}dz\int_0^\infty dt[\xi_0(P^2)\,\delta(t)+\eta_0(z,t;P^2)] \times[q^2+z(q\cdot P)+m^2+P^2/4+t]^{-2}. \tag{2.2}$$

This representation is essentially the same as the one that was first introduced by Wanders.[5] Ida and Maki[6] have proved that all the eigenfunctions of the kernel in the abovementioned Wick's equation can be expressed in the form (2.2).

Inserting (2.1) and (2.2) into (1.4), and transforming the integral over q' into Feynman's param-

[4] G. C. Wick, Phys. Rev. **96**, 1124 (1954).
[5] G. Wanders, Helv. Phys. Acta **30**, 417 (1957).
[6] M. Ida and K. Maki, Progr. Theoret. Phys. (Kyoto) **26**, 470 (1961).

eter integral, we have the following system of equations:

$$\eta_0(z, t; P^2) = -\lambda\xi_0(P^2)\int_{-1}^{1} dz' k_0(z, t; z', 0; P^2) - \lambda\int_{-1}^{1} dz' \int_0^\infty dt' k_0(z, t; z', t'; P^2)\eta_0(z', t'; P^2), \tag{2.3}$$

$$\xi_0(P^2) + \int_0^\infty dt \eta_0(z, t; P^2) = 1. \tag{2.4}$$

where k_0 is defined by

$$\begin{aligned} k_0(z, t; z', t'; P^2) = \theta\{t\rho(z, z') - t' - \mu^2 - 2\mu \\ \times [t' + m^2 + (1 - z'^2)P^2/4]^{1/2}\} \\ \times (2t)^{-1}[t\rho(z, z') - t' + \mu^2] \\ \times [t\rho(z, z') + m^2 + (1 - z'^2)P^2/4]^{-1} \\ \times \{t\rho(z, z') - t' - \mu^2 - 2\mu \\ \times [t' + m^2 + (1 - z'^2)P^2/4]^{1/2}\}^{-1/2} \\ \times \{t\rho(z, z') - t' - \mu^2 + 2\mu \\ \times [t' + m^2 + (1 - z'^2)P^2/4]^{1/2}\}^{-1/2}, \end{aligned} \tag{2.5}$$

with the abbreviation

$$\rho(z, z') = (1 \pm z')/(1 \pm z), \quad \text{for} \quad z \lesseqgtr z'. \tag{2.6}$$

We immediately see from (2.5) that k_0 is positive definite. The independence of the second term in the left-hand side of (2.4) on z follows from (2.3), if the integral $\int_0^\infty dt\, k_0(z, t; z', t'; P^2)$ is independent of z. But this is really the case, as is seen by transforming the integration variable t into $t\rho(z, z')$.

We see from (2.5) that k_0 is not bounded. In order to obtain an integral equation with a bounded kernel, we iterate (2.3). Then we have

$$\begin{aligned} \eta_0(z, t; P^2) = -\lambda\xi_0(P^2)\int_{-1}^{1} dz' \\ \times [k_0(z, t; z', 0; P^2) - \lambda k_0^{(2)}(z, t; z', 0; P^2)] \\ + \lambda^2\int_{-1}^{1} dz' \int_0^\infty dt' k_0^{(2)}(z, t; z', t'; P^2)\eta_0(z', t'; P^2), \end{aligned} \tag{2.7}$$

where $k_0^{(2)}$ is the iterated kernel defined by

$$\begin{aligned} k_0^{(2)}(z, t; z', t') = \int_{-1}^{1} dz'' \int_0^\infty dt'' k_0(z, t; z'', t'') \\ \times k_0(z'', t''; z', t'). \end{aligned} \tag{2.8}$$

Equation (2.7) is a regular integral equation to which we can apply the Fredholm solution formula. In fact, if we transform the variable t into σ by $t = \tau(z, \sigma)$, where

$$\tau(z, \sigma) = (m^2/4)(1 - z^2)\sigma^4(1 - \sigma)^{-4}, \tag{2.9}$$

the infinite region $-1 \leq z \leq 1$, $0 \leq t < \infty$ is transformed into the finite region $-1 \leq z \leq 1$, $0 \leq \sigma \leq 1$ and it is proved that

$$\begin{aligned} 0 \leq [\partial\tau(z, \sigma)/\partial\sigma]k_0^{(2)}(z, \tau(z, \sigma); z', \tau(z', \sigma'); P^2) \\ < 11\pi \frac{(\mu^2 + m^2 + P^2/4)\{m^{1/2} + [\mu^2 + 2\mu(m^2 + P^2/4)^{1/2}]^{1/4}\}^2}{m^{1/2}\mu(m^2 + P^2/4)^{5/4}[\mu^2 + 2\mu(m^2 + P^2/4)^{1/2}]^{3/2}}, \\ \text{for} \quad -1 \leq z, z' \leq 1, \quad 0 \leq \sigma, \sigma' \leq 1. \end{aligned} \tag{2.10}$$

The proof is given in the Appendix. This inequality means that if $\mu > 0$ and $-4m^2 < P^2 \leq 0$, the following Fredholm series associated with (2.7) are convergent [uniformly for (2.12)] for any value of λ:

$$D_0(P^2) \equiv 1 + \sum_{n=1}^{\infty} \frac{(-\lambda^2)^n}{n!} \int (dv)_n \begin{vmatrix} k_0^{(2)}(1, 1) & \cdots & k_0^{(2)}(1, n) \\ \cdots & \cdots & \cdots \\ k_0^{(2)}(n, 1) & \cdots & k_0^{(2)}(n, n) \end{vmatrix}, \tag{2.11}$$

$$\begin{aligned} D_0(z, t; z', t'; P^2) \equiv k_0^{(2)}(z, t; z', t') \\ + \sum_{n=1}^{\infty} \frac{(-\lambda^2)^n}{n!} \int (dv)_n \begin{vmatrix} k_0^{(2)}(z, t; z', t')k_0^{(2)}(z, t; 1) & \cdots & k_0^{(2)}(z, t; n) \\ k_0^{(2)}(1; z', t')k_0^{(2)}(1, 1) & \cdots & k_0^{(2)}(1, n) \\ \cdots & \cdots & \cdots \\ k_0^{(2)}(n; z', t')k_0^{(2)}(n, 1) & \cdots & k_0^{(2)}(n, n) \end{vmatrix}, \end{aligned} \tag{2.12}$$

where

$$k_0^{(2)}(i, j) = k_0^{(2)}(z_i, t_i; z_j, t_j),$$

$$\int (dv)_n = \int_{-1}^{1} dz_1 \int_0^{\infty} dt_1 \cdots \int_{-1}^{1} dz_n \int_0^{\infty} dt_n,$$

and we have suppressed the argument P^2 in $k_0^{(2)}$. The solution to the system of equations (2.4) and (2.7) can be easily written down in terms of these functions. The result is as follows:

$$\eta_0(z, t; P^2) = \int_{-1}^{1} dz'\ \Delta_0(z, t; z', 0; P^2)/\Delta_0(P^2), \quad (2.13)$$

$$\xi_0(P^2) = D_0(P^2)/\Delta_0(P^2), \quad (2.14)$$

where

$$\Delta_0(z, t; z', t'; P^2) = -\lambda\, D_0(P^2)k_0(z, t; z', t'; P^2)$$

$$+ \lambda^2\, D_0(z, t; z', t'; P^2) - \lambda^3 \int_{-1}^{1} dz'' \int_0^{\infty} dt''$$

$$\times\, D_0(z, t; z'', t''; P^2)k_0(z'', t''; z', t'; P^2), \quad (2.15)$$

$$\Delta_0(P^2) = D_0(P^2) + \int_0^{\infty} dt \int_{-1}^{1} dz'\ \Delta_0(z, t; z', 0; P^2). \quad (2.16)$$

We have also proved that

$$[\partial\tau(z, \sigma)/\partial\sigma] \int_{-1}^{1} dz' k_0(z, \tau(z, \sigma); z', 0)$$

is a bounded function of z and σ in the region $-1 \leq z \leq 1$, $0 \leq \sigma \leq 1$, provided that $-P^2 \neq 2m^2 + m\mu$. From this and (2.15) it follows that

$$[\partial\tau(z, \sigma)/\partial\sigma] \int_{-1}^{1} dz'\ \Delta_0(z, \tau(z, \sigma); z', 0; P^2) \quad (2.17)$$

is a bounded function of z and σ in the region $-1 \leq z \leq 1$, $0 \leq \sigma \leq 1$, unless $-P^2 = 2m^2 + m\mu$.

As was mentioned in Sec. 1, mass of the scalar deuteron corresponds to a pole of $F(q, P)$, namely, a pole of η_0 and/or ξ_0. Therefore, because of (2.13) and (2.14), the mass m_d is determined by

$$\Delta_0(-m_d^2) = 0. \quad (2.18)$$

We further see from (2.2), (2.13), and (2.14) that $f(q, D)$, which is defined by (1.6), is given by

$$f(q, D) = \frac{1}{2} \int_{-1}^{1} dz \int_0^{\infty} dt[\gamma_0\, \delta(t) + \zeta_0(z, t)]$$

$$\times\, [q^2 + z(q \cdot D) + m^2 - m_d^2/4 + t]^{-2}, \quad (2.19)$$

with

$$\zeta_0(z, t) = \int_{-1}^{1} dz'\ \Delta_0(z, t; z', 0; -m_d^2)/\Delta_0'(-m_d^2), \quad (2.20)$$

$$\gamma_0 = D_0(-m_d^2)/\Delta_0'(-m_d^2), \quad (2.21)$$

where $\Delta_0'(P^2)$ denotes $d\Delta_0(P^2)/dP^2$. Then it follows from (2.18) and (2.16) that

$$\gamma_0 + \int_0^{\infty} dt\zeta_0(z, t) = 0. \quad (2.22)$$

As a result of this relation, $f(q, D)$ behaves like q^{-6} as $q \to \infty$. This is necessary for the convergence of the integral in the normalization condition (1.8).

Here it should be mentioned that only those roots of (2.18) for which $\Delta_0(z, t; z', t'; -m_d^2)$ does not identically vanish correspond to the bound states. The reason for this remark is as follows: Suppose that $D_0(P^2) = 0$ for a certain value of P^2. Then $D_0(z, t; z', t'; P^2)$ for fixed z' and t' is an eigenfunction of $k_0^{(2)}$ belonging to the eigenvalue λ^2, so it is also an eigenfunction of k_0 belonging to the eigenvalue λ or $-\lambda$. If λ is the eigenvalue, $\Delta_0(z, t; z', t'; P^2)$ identically vanishes as is seen from (2.15). In this case, though we have $\Delta_0(P^2) = 0$, this value of P^2 is not a pole of η_0 or ξ_0.

The normalization condition (1.8) now becomes, by the insertion of (2.19) and the use of (2.22),

$$|N|^{-2} = \frac{-1}{32\pi^2} \int_{-1}^{1} dz \int_0^{\infty} dt\zeta_0(z, t)$$

$$\times \ln \frac{t + m^2 - (1 - z^2)m_d^2/4}{m^2 - (1 - z^2)m_d^2/4}. \quad (2.23)$$

The integral on the right-hand side is evidently convergent by virtue of (2.17). Therefore, the Bethe-Salpeter wavefunction given by (1.5) is finite. Unfortunately, however, we cannot say anything about the sign of the right-hand side of (2.23). We will show in Sec. 5 that the right-hand side of (2.23) is positive for all the eigenvalues in the non-relativistic limit.

Since the series (2.11) and (2.12) are always convergent, the expansions of $\Delta_0(P^2)$ and $\Delta_0(z, t; z', t'; P^2)$ in powers of λ are also always convergent. If the convergence is sufficiently fast, one can have an approximate solution by retaining the first few terms in those expansions. The accuracy of the approximation can be estimated with the aid of (2.10). If we retain terms in λ^0 and λ^1 as the first approximation, we have from (2.15) and (2.16)

$$\Delta_0(z, t; z', t'; P^2) = -\lambda k_0(z, t; z', t'; P^2), \quad (2.24)$$

$$\Delta_0(P^2) = 1 - \lambda \int_0^{\infty} dt \int_{-1}^{1} dz' k_0(z, t; z', 0; P^2), \quad (2.25)$$

therefore the mass m_d is determined by

$$1 = \lambda \int_0^{\infty} dt \int_{-1}^{1} dz' k_0(z, t; z', 0; -m_d^2). \quad (2.26)$$

This equation is found to be equivalent to that of Blankenbecler and Cook[1] if the self-energy part of the proton is neglected in the latter.

When we want to obtain the eigenvalue λ under the condition that $m_d \ll m$ and $m_d \ll \mu$, we have another approximation method. In this case we put $P^2 = 0$ as the first approximation. Then we see from (2.5) that the kernel k_0 has the following form:

$$k_0(z, t; z', t'; 0) = f(t, t', \rho(z, z')).$$

Inserting this into (2, 3) and integrating the both sides over z, we have, because of (2.6),

$$\bar{\eta}(t) = -\lambda\xi(0)\bar{k}(t, 0) - \lambda \int_0^\infty dt'\bar{k}(t, t')\bar{\eta}(t'), \quad (2.27)$$

where

$$\bar{\eta}(t) \equiv \frac{1}{2}\int_{-1}^{1} dz\eta_0(z, t; 0),$$

$$\bar{k}(t, t') \equiv 2\int_1^\infty d\rho\rho^{-2}f(t, t', \rho).$$

Equation (2.27) is a one-dimensional equation. Moreover, if $\bar{k}$ is calculated explicitly, it is found that (2.27) can be reduced to an integral equation of Volterra type, which is solved by the Neumann series. This approximation is essentially the same as that of Thirring *et al.*[7]

3. DISPERSION RELATION FOR THE DEUTERON-PROTON-NEUTRON VERTEX FUNCTION

We consider the function

$$\Gamma(-(D - n)^2) \equiv 2V(n_0 D_0)^{1/2}\langle n \,|j_p(0)|\, D\rangle, \quad (3.1)$$

where $j_p(x) \equiv (m^2 - \Box)\varphi_p(x)$ and $|n\rangle$ is the single neutron state with four-momentum n satisfying $n^2 = -m^2$. Γ is related to the Bethe-Salpeter wave-function χ by

$$\Gamma(-(D - n_j)^2) = i\int d^4x_2 \exp(-inx_2)$$

$$\times [(m^2 - \Box_1)(m^2 - \Box_2)\chi(x_1, x_2; D)]_{x_1=0}. \quad (3.2)$$

Inserting the Fourier-integral representation (1.5) for χ into (3.2), we have

$$\Gamma(-(D - n)^2) = N^*V(\tfrac{1}{2}D - n, D), \quad (3.3)$$

where

$$V(q, D) \equiv [(\tfrac{1}{2}D + q)^2 + m^2] \times [(\tfrac{1}{2}D - q)^2 + m^2]f(q, D). \quad (3.4)$$

Since $f(q, D)$ satisfies the homogeneous version of (1.4), we have

$$V(q, D) = \int d^4q'G(q, q'; D)f(q', D). \quad (3.5)$$

Inserting (2.1) and (2.19) into the right-hand side and carrying out the integration over q' by means of the Feynman's method, we have

$$V(q, D) = \lambda\int_{-1}^{1} dz\int_0^\infty dt\int_0^\infty dt'k_0(z, t; z, t'; -m_d^2) \times [\gamma_0\,\delta(t') + \zeta_0(z, t')]t \times [q^2 + z(q\cdot D) + m^2 - m_d^2/4 + t]^{-1}. \quad (3.6)$$

Using this equation, we can easily rewrite (3.3) as

$$\Gamma(x) = \frac{1}{\pi}\int_{m^2}^\infty dx' \frac{\rho(x')}{x' - x}, \quad (3.7)$$

where

$$\rho(x') \equiv \pi N^*\lambda\int_{-1}^{1} dz\int_0^\infty dt'\tfrac{1}{2}(1 + z)(x' - m^2) \times k_0(z, \tfrac{1}{2}(1 + z)(x' - m^2); z, t'; -m_d^2) \times [\gamma_0\,\delta(t') + \zeta_0(z, t')]. \quad (3.8)$$

Convergence of the integral in (3.7) can be easily verified by the use of (2.5) and (2.17).

Now, the actual lower limit of the integral (3.7), which we denote by a, is not m^2, but larger than m^2. We see from (2.5) that the k_0 in (3.8) has the factor $\theta[x' - f(z, t')]$, where

$$f(z, t') = m^2 + 2(1 + z)^{-1} \times \{t' + \mu^2 + 2\mu[t' + m^2 - (1 - z^2)m_d^2/4]^{1/2}\}.$$

Therefore a is the minimum value of $f(z, t')$ in the region $-1 \le z \le 1$, $0 \le t' < \infty$. This minimum value is as follows:

$$a = (m + \mu)^2, \quad \text{when} \quad m_d^2 < 2m^2 + m\mu,$$

$$a = m^2 + (2m^2)^{-1}\mu m_d \times [\mu m_d + (4m^2 - \mu^2)^{1/2}(4m^2 - m_d^2)^{1/2}],$$

when $4m^2 > m_d^2 > 2m^2 + m\mu$.
The latter is the well-known anomalous threshold.

We have thus proved that, within the ladder approximation, $\Gamma(x)$ satisfies the dispersion relation without subtraction which was assumed by Blankenbecler and Cook.[1]

The renormalized deuteron-proton-neutron coupling constant Γ_d is defined as $\Gamma(m^2)$. Making x equal to m^2 in (3.7), we have

$$\Gamma_d = N^*\lambda\int_{-1}^{1} dz\int_0^\infty dt\int_0^\infty dt'k_0(z, t; z, t'; -m_d^2) \times [\gamma_0\,\delta(t') + \zeta_0(z, t')]. \quad (3.9)$$

[7] K. Baumann and W. Thirring, Nuovo cimento **18**, 357 (1960); K. Baumann, P. G. O. Freund, and W. Thirring, *ibid.* **18**, 906 (1960).

Using the system of integral equations satisfied by γ_0 and ζ_0, which is the homogeneous version of the system of equations (2.3) and (2.4), we easily obtain from (3.9) $\Gamma_d = N^*\gamma_0$. If we neglect ζ_0 in the right-hand side of (3.9), and replace $N^*\gamma_0$ by Γ_d, we have again the same approximate equation as (2.26):

$$1 = \lambda \int_{-1}^{1} dz \int_0^\infty dt k_0(z, t; z, 0; -m_d^2).$$

4. VECTOR SOLUTIONS IN THE LADDER APPROXIMATION

We first consider the transversal case. In this case we have to solve the integral equation (1.12) for $F_t(q, P)$. As in the scalar case we write $F_t(q, P)$ as

$$F_t(q, P) = \frac{1}{2}\int_{-1}^{1} dz \int_0^\infty dt[\xi_1(P^2)\ \delta(t) + \eta_1(z, t; P^2)] \times [q^2 + z(q\cdot P) + m^2 + P^2/4 + t]^{-2}. \quad (4.1)$$

If we insert this and the ladder approximation (2.1) into (1.12) and put

$$k_1(z, t; z', t'; P^2) = \{[t' + m^2 + (1 - z'^2)P^2/4 - \mu^2] \times [t\rho(z, z') + m^2 + (1 - z'^2)P^2/4]^{-1} + 2\mu^2[t\rho(z, z') - t' + \mu^2]^{-1}\}k_0(z, t; z', t'; P^2), \quad (4.2)$$

we obtain that system of integral equations for ξ_1 and η_1 which is obtained from the system of equations (2.3) and (2.4) just by replacing every subscript 0 by 1. We further find by the use of (4.2) and (2.5) that

$$0 \leq k_1(z, t; z', t'; P^2) < k_0(z, t; z', t'; P^2). \quad (4.3)$$

Consequently the analogue of the iterated integral equation (2.7) is again regular. Therefore the system of integral equations satisfied by ξ_1 and η_1 can be solved by exactly the same method as was used in solving (2.3) and (2.4), and the solution is given by the expressions which are obtained from (2.11)–(2.16) just by replacing every subscript 0 by 1. And exactly in the same way as in the scalar case, we have the following results: the mass of the transversal deuteron m_d is determined by

$$\Delta_1(-m_d^2) = 0. \quad (4.4)$$

$f_t(q, D)$ which is defined by (1.17) is expressed as

$$f_t(q, D) = \frac{1}{2}\int_{-1}^{1} dz \int_0^\infty dt[\gamma_1\ \delta(t) + \zeta_1(z, t)] \times [q^2 + z(q\cdot D) + m^2 - m_d^2/4 + t]^{-2}, \quad (4.5)$$

where ζ_1 and γ_1 are given by the expressions which are obtained, respectively, from (2.20) and (2.21) by replacing every subscript 0 by 1. Analogous to (2.22), we have

$$\gamma_1 + \int_0^\infty dt\zeta_1(z, t) = 0. \quad (4.6)$$

Differently from the scalar case, (4.6) is not enough to make the normalization integral in (1.18) convergent because of the factor $(e^{(\alpha)}\cdot q)^2$ in the integrand. However, we have one more relation in the following way: Using (4.2) and (2.5), we can derive

$$\int_0^\infty dt\ tk_1(z, t; z', t'; P^2) = [2\rho(z, z')]^{-1}. \quad (4.7)$$

If we multiply (2.3), with subscripts 1 in place of 0, by t, and integrate over t, we have on account of (4.7) and (2.4), with subscripts 1 in place of 0,

$$\int_0^\infty dt\ t\eta_1(z, t; P^2) = -\lambda \int_{-1}^{1} dz'[2\rho(z, z')]^{-1}. \quad (4.8)$$

Multiplying both sides of this equation by $m_d^2 + P^2$ and making P^2 tend to $-m_d^2$, we have

$$\int_0^\infty dt\ t\zeta_1(z, t) = 0. \quad (4.9)$$

Because of (4.6) and (4.9), $f_t(q, D)$ given by (4.5) behaves like q^{-8} as $q \to \infty$. Therefore, if we insert (4.5) into (1.18), the integral over q is convergent and we have

$$|N|^{-2} = \frac{1}{64\pi^2}\int_{-1}^{1} dz \int_0^\infty dt\zeta_1(z, t) \times [t + m^2 - (1 - z^2)m_d^2/4] \times \ln\frac{t + m^2 - (1 - z^2)m_d^2/4}{m^2 - (1 - z^2)m_d^2/4}. \quad (4.10)$$

After a careful examination[8] we have found that the integral in (4.10) is convergent. We will show in the next section that the right-hand side of (4.10) is always positive in the nonrelativistic limit.

Next we consider the longitudinal case. The integral equation which we have to solve is (1.13). In this case we put

$$F_l(q, P) = \frac{1}{2P^2}\int_{-1}^{1} dz \times \int_0^\infty dt \frac{\eta_-(z, t; P^2)}{[q^2 + z(q\cdot P) + m^2 + P^2/4 + t]^2}. \quad (4.11)$$

[8] ζ_1 satisfies the integral equation which is obtained from (2.3) by replacing η_0 by ζ_1, k_0 by k_1, and ξ_0 by γ_1. It also satisfies the same boundedness condition as (2.17). Using these facts and the expression of k_1, we can prove that $|\int_0^{t'} dt\ t\zeta_1(z, t)| < Ct'^{-1/4}$, where C is a constant. From this follows the convergence of the integral in (4.10).

Then (1.13) is transformed into

$$\eta_-(z, t; P^2) = \delta(z+1) - \delta(z-1) - \lambda \int_{-1}^{1} dz' \times \int_0^\infty dt' k_0(z, t; z', t'; P^2)\eta_-(z', t'; P^2), \quad (4.12)$$

where k_0 is given by (2.5). We immediately see from (2.5) that

$$k_0(z, t; z', t'; P^2) = k_0(-z, t; -z', t'; P^2). \quad (4.13)$$

From this and (4.12) it follows that $\eta_-(z, t; P^2)$ is an odd function of z. In fact, in deriving (4.12), we have dropped a term which vanishes by virtue of the oddness of η_-.

If we iterate (4.12), we have an integral equation with the iterated kernel $k_0^{(2)}$, so we can immediately write down the solution in terms of the functions (2.11) and (2.12). The result is as follows:

$$\eta_-(z, t; P^2) = \delta(z+1) - \delta(z-1) - \lambda \int_0^\infty dt'[k_0(z, t; -1, t'; P^2) - k_0(z, t; 1, t'; P^2)] + \lambda^2 D_-(z, t; P^2)/D_0(P^2), \quad (4.14)$$

where

$$D_-(z, t; P^2) \equiv \int_{-1}^{1} dz' \int_0 dt' D_0(z, t; z', t'; P^2) \times \{\delta(z'+1) - \delta(z'-1) - \lambda \int_0^\infty dt''[k_0(z', t'; -1, t''; P^2) - k_0(z', t'; 1, t''; P^2)]\}. \quad (4.15)$$

The mass of the longitudinal deuteron is therefore determined by

$$D_0(-m_d^2) = 0 \quad (4.16)$$

and $f_l(q, D)$, which is defined by (1.20), is given by

$$f_l(q, D) = -(2m_d^2)^{-1} \int_{-1}^{1} dz \int_0^\infty dt \zeta_-(z, t) \times [q^2 + z(q\cdot D) + m^2 - m_d^2/4 + t]^{-2}, \quad (4.17)$$

where

$$\zeta_-(z, t) = \lambda^2 D_-(z, t; -m_d^2)/D_0'(-m_d^2). \quad (4.18)$$

The same remark as in the scalar case applies also to this case: Only those roots of (4.16) for which $D_-(z, t; -m_d^2)$ does not identically vanish correspond to the bound states.

Now we have

$$\int_0^\infty dt \zeta_-(z, t) = 0, \quad (4.19)$$

because this integral is independent of z whereas $\zeta_-(z, t)$ is an odd function of z. Consequently $f_l(q, D)$ behaves like q^{-6} as $q \to \infty$. Therefore, if we insert (4.17) into the normalization condition (1.21), the integral over q converges, and we have

$$|N|^{-2} = -\frac{1}{64\pi^2 m_d^2} \int_{-1}^{1} dz \int_0^\infty dt z \zeta_-(z, t) \times \ln \frac{t + m^2 - (1-z^2)m_d^2/4}{m^2 - (1-z^2)m_d^2/4}. \quad (4.20)$$

Since ζ_- satisfies the same boundedness condition as (2.17), the integral in (4.20) is obviously convergent.

The present longitudinal vector solution belongs to the S-state solution of Wick[4] and Cutkosky,[9] because $f_l(q, D)$ is a function of $\mathbf{q}^2$ and q_0 alone in the rest system of the deuteron. But, since $f_l(q, D)$ is an odd function of q_0, the present solution is the abnormal solution with odd value of the quantum number κ in reference 9. In the nonrelativistic limit the longitudinal solution does not exist, because the integral equation (4.12) reduces to the one of the Volterra type which has no eigenvalues.

5. NONRELATIVISTIC LIMIT

In order to make the meaning of the normalization condition clear, we investigate in this section the nonrelativistic limit of the equations obtained in Secs. 2 and 4. For this purpose it is convenient to put $P^2 = -4(m^2 - \alpha^2)$. In the nonrelativistic limit we make m tend to infinity, leaving μ and α finite.

First we consider the scalar case. The problem is to find out the nonrelativistic limit of (2.3) and (2.4). This problem has been already solved by Wanders,[5] but his procedure was very complicated. Because our procedure is much simpler, it will be worthwhile to state it here. We first rewrite the expression of k_0 (2.5) as

$$k_0(z, t; z', t'; P^2) = (2\mu)^{-1}(m^2 - \alpha^2)^{-1/2}\theta[\epsilon(z')^2 - z'^2] \times \theta\{t\rho(z, z') - t' - \mu^2 - 2\mu \times [t' + \alpha^2 + (m^2 - \alpha^2)z'^2]^{1/2}\} \times (2t)^{-1}[t\rho(z, z') - t' + \mu^2] \times [\epsilon(z')^2 - z'^2]^{-1/2} \times [t\rho(z, z') + \alpha^2 + (m^2 - \alpha^2)z'^2]^{-1}, \quad (5.1)$$

[9] R. E. Cutkosky, Phys. Rev. **96**, 1135 (1954).

where

$$\epsilon(z')^2 = [4\mu^2(m^2 - \alpha^2)]^{-1} \times \{[t\rho(z, z') - t' - \mu^2]^2 - 4\mu^2(t' + \alpha^2)\}.$$

We assume that $m^2 \gg t, t', \mu^2, \alpha^2$. Then we find that $\epsilon(z') \ll 1$. Therefore, because of the first θ function in (5.1), k_0 is different from zero only when z' is in a very small interval around $z' = 0$. We also see that only the last two factors in (5.1) rapidly vary with z'. Therefore we can put $z' = 0$ in the remaining factors, and also can replace $\epsilon(z')$ and $\rho(z, z')$ in the last two factors by $\epsilon(0) \equiv \epsilon$ and $\rho(z, 0)$ respectively. Thus we have in the nonrelativistic limit

$$k_0(z, t; z', t'; P^2) = (2\mu)^{-1}(m^2 - \alpha^2)^{-1/2}\,\delta(z') \times \theta[t\rho(z, 0) - t' - \mu^2 - 2\mu(t' + \alpha^2)^{1/2}] \times [t\rho(z, 0) - t' + \mu^2](2t)^{-1} \int_{-\epsilon}^{\epsilon} dz'' \times [t\rho(z, 0) + \alpha^2 + (m^2 - \alpha^2)z''^2]^{-1}(\epsilon^2 - z''^2)^{-1/2}.$$

The integration is easily carried out, yielding

$$k_0(z, t; z', t'; P^2) = (\pi/2m)[t\rho(z, 0) + \alpha^2]^{1/2} \times t^{-1}\theta[t\rho(z, 0) - t' - \mu^2 - 2\mu(t' + \alpha^2)^{1/2}]\,\delta(z'). \quad (5.2)$$

We insert this into (2.3), set $z = 0$ in both sides, and transform the variables as follows:

$$t = x^2 - \alpha^2,$$

$$\eta_0(0, t; P^2)/\xi_0(P^2) = (2x)^{-1}\omega_0(x, \alpha^2). \quad (5.3)$$

Then we have the following integral equation:

$$\omega_0(x, \alpha^2) = -l(x^2 - \alpha^2)\left[\theta(x - \mu - \alpha) + \theta(x - 2\mu - \alpha)\int_{\alpha+\mu}^{x-\mu} dx'\omega_0(x', \alpha^2)\right], \quad (5.4)$$

where $l \equiv \pi\lambda/m$. On the other hand, (2.4) is transformed by (5.3) into

$$\xi_0(P^2) = 1/J_0(\alpha^2), \quad (5.5)$$

where

$$J_0(\alpha^2) \equiv 1 + \int_{\mu+\alpha}^{\infty} dx\omega_0(x, \alpha^2). \quad (5.6)$$

Equation (5.4) is a special case of the integral equation derived by Bertocchi *et al.*[10] for the Laplace transform of the Schrödinger wavefunction. This proves that the Bethe-Salpeter equation gives the ordinary Schrödinger equation with the Yukawa potential in the nonrelativistic limit. The Neumann series associated with (5.4) is always convergent. In fact, for any finite value of x, a finite number of iterations suffices for calculating exact value of ω_0.

On account of (5.5), the binding energy is determined by

$$J_0(\alpha_0^2) = 0, \quad (5.7)$$

where we have put $\alpha_0^2 = m^2 - m_d^2/4 = (mB)^{1/2}$, B being the binding energy. The function

$$\zeta_0(z, t) \equiv [(m_d^2 + P^2)\eta_0(z, t; P^2)]_{P^2=-m_d^2}$$

now becomes

$$\zeta_0(0, t) = 2\omega_0(x, \alpha_0^2)/[xJ_0'(\alpha_0^2)]. \quad (5.8)$$

Now, the logarithm in the normalization condition (2.23) is found to be appreciably different from zero only for $z \approx 0$ in the nonrelativistic limit. Therefore the integral in (2.23) can be expressed in terms of $\zeta_0(0, t)$, which is given by (5.8). Indeed it is easily found that (2.23) becomes, in the nonrelativistic limit,

$$|N|^{-2} = -[4\pi m J_0'(\alpha_0^2)]^{-1}\int_{\mu+\alpha_0}^{\infty} dx(x - \alpha_0)\omega_0(x, \alpha_0^2) \quad (5.9)$$

In order to see the meaning of the above equation, we introduce the function

$$u_0(r, \alpha) \equiv e^{-\alpha r} + \int_{\mu+\alpha}^{\infty} dx\omega_0(x, \alpha^2)e^{-xr}. \quad (5.10)$$

Then it follows from (5.4) that

$$\left(\frac{d^2}{dr^2} - \alpha^2 + l\frac{e^{-\mu r}}{r}\right)u_0(r, \alpha) = 0. \quad (5.11)$$

This means that u_0 is the S-state radial wavefunction in the Schrödinger theory. From (5.10) and (5.6) we have

$$J_0(\alpha^2) = u_0(0, \alpha). \quad (5.12)$$

Therefore (5.7) is nothing but the ordinary eigenvalue condition. From (5.10), (5.7), and (5.6) we have

$$u_0'(0, \alpha_0) = -\int_{\mu+\alpha_0}^{\infty} dx(x - \alpha_0)\omega_0(x, \alpha_0^2), \quad (5.13)$$

where the prime means the derivative with respect to r. We further introduce the function $v(r, \alpha) \equiv \partial u_0(r, \alpha)/\partial\alpha^2$. Then, differentiating (5.11) with respect to α^2, we have

$$\left(\frac{d^2}{dr^2} - \alpha^2 + l\frac{e^{-\mu r}}{r}\right)v(r, \alpha) = u_0(r, \alpha). \quad (5.14)$$

[10] L. Bertocchi, C. Ceolin, and M. Tonin, Nuovo cimento **18**, 770 (1960).

If we subtract (5.14) multiplied by u_0 from (5.11) multiplied by v, and integrate the result over r, we have, because $u_0(0, \alpha_0) = 0$,

$$J_0'(\alpha_0^2) = \int_0^\infty dr \frac{u_0(r, \alpha_0^2)^2}{u_0'(0, \alpha_0)}. \tag{5.15}$$

In obtaining this we have used the relation $v(0, \alpha_0) = J_0'(\alpha_0^2)$ which follows from (5.12) and the definition of v. Inserting (5.13) and (5.15) into (5.9), we have

$$|N|^{-2} = u_0'(0, \alpha_0)^2 \left[4\pi m \int_0^\infty dr u_0(r, \alpha_0)^2 \right]^{-1}. \tag{5.16}$$

The right-hand side of this equation is obviously positive.

If we introduce the normalized S-state wavefunction $\psi_0(r)$, (5.16) becomes $|N|^{-2} = \psi(0)^2/m$. The same result is obtained if we calculate $|N|$ from the definition (1.7) by the use of

$$\langle 0 \, | \varphi_p(\mathbf{x}_1)\varphi_n(\mathbf{x}_2) | \, \mathbf{r}_p, \mathbf{r}_n \rangle = (2V^2 m)^{-1} \times \sum_{p,n} \exp\left[i\mathbf{p}(\mathbf{x}_1 - \mathbf{r}_p) + i\mathbf{n}(\mathbf{x}_2 - \mathbf{r}_n) \right], \tag{5.17}$$

$$\langle \mathbf{r}_p, \mathbf{r}_n \mid D \rangle = V^{-1/2} \times \exp\left[i\mathbf{D} \cdot \tfrac{1}{2}(\mathbf{r}_p + \mathbf{r}_n) \right] \psi_0(|\mathbf{r}_p - \mathbf{r}_n|). \tag{5.18}$$

The transversal vector case is treated in a similar way. We therefore give only the results in the following. In the nonrelativistic limit, the integral equation for η_1, which is (2.3) with subscripts 1 in place of 0, reduces to

$$\omega_1(x, \alpha^2) = \frac{-l}{x^2 - \alpha^2} \left[\theta(x - \mu - \alpha) \frac{x^2 + \alpha^2 - \mu^2}{2x\alpha} + \theta(x - 2\mu - \alpha) \times \int_{\mu+\alpha}^{x-\mu} dx' \frac{x^2 + x'^2 - \mu^2}{2xx'} \omega_1(x', \alpha^2) \right], \tag{5.19}$$

where

$$t = x^2 - \alpha^2,$$

$$\eta_1(0, t; P^2)/\xi_1(P^2) = \alpha(2x^2)^{-1}\omega_1(x, \alpha^2). \tag{5.20}$$

Equation (5.19) is again a special case of the equation given by Bertocchi *et al.*[10] for the P-state Schrödinger wavefunction. The binding energy is determined by

$$1 + \alpha_0 \int_{\mu+\alpha_0}^\infty dx \, x^{-1}\omega_1(x, \alpha_0^2) = 0. \tag{5.21}$$

As a result of (5.19), the function

$$u_1(r, \alpha) \equiv [1 + (\alpha r)^{-1}]e^{-\alpha r} + \int_{\mu+\alpha}^\infty dx \omega_1(x, \alpha^2)[1 + (xr)^{-1}]e^{-xr} \tag{5.22}$$

satisfies the Schrödinger equation for the P-state radial wavefunction

$$\left(\frac{d^2}{dr^2} - \frac{2}{r^2} - \alpha^2 + l\frac{e^{-\mu r}}{r} \right) u_1(r, \alpha) = 0. \tag{5.23}$$

The normalization condition (4.10) is then written in terms of the function u_1 as

$$|N|^{-2} = 3\{[u_1(r, \alpha_0)/r^2]_{r=0}\}^2 \times \left\{ 4\pi m \int_0^\infty dr u_1(r, \alpha_0)^2 \right\}^{-1}. \tag{5.24}$$

The right-hand side is again positive. If we calculate $|N|$ from the definition (1.15) by the use of (5.17) and the P-state analog of (5.18), we have the same result as (5.24).

6. THE LADDER-CHAIN APPROXIMATION FOR THE NUCLEON-ANTINUCLEON CASE

In this section we consider the bound state of the nucleon and antinucleon. In this case it is possible that a nucleon-antinucleon pair annihilates to form a meson and vice versa. The simplest approximation to take this process into account is to put

$$G(q, q'; P) = -i\lambda\pi^{-2}[(q - q')^2 + \mu^2]^{-1} - ig_0^2(2\pi)^{-4}(P^2 + \mu_0^2)^{-1}, \tag{6.1}$$

where μ_0 and g_0 are the unrenormalized mass of the meson and unrenormalized coupling constant. We confine ourselves to the scalar case. Then the inhomogeneous Bethe-Salpeter equation (1.4) still holds. The homogeneous version of (1.4) with (6.1) has been solved approximately by Okubo and Feldman[2] for the case $\mu = \mu_0 = 0$. If we insert (6.1) into (1.4), we easily see that the solution can be written as

$$F(q, P) = F_0(q, P)[1 - g_0^2(P^2 + \mu_0^2)^{-1}\Sigma(P^2)]^{-1}, \tag{6.2}$$

where $F_0(q, P)$ is the solution of the integral equation

$$F_0(q, P) = [(\tfrac{1}{2}P + q)^2 + m^2]^{-1}[(\tfrac{1}{2}P - q)^2 + m^2]^{-1} \times \left\{ 1 - i\lambda\pi^{-2} \int d^4q' [(q - q')^2 + \mu^2]^{-1} F_0(q', P) \right\}, \tag{6.3}$$

and $\Sigma(P^2)$ is defined by

$$\Sigma(P^2) = -i(2\pi)^{-4} \int d^4q F_0(q, P). \tag{6.4}$$

Equation (6.3) is nothing but the equation in the ladder approximation, so its solution has been given in Sec. 2.

Now we introduce the unrenormalized meson propagator including radiative corrections, and denote it by $\Delta_m'(P)$. If we calculate it in the same approximation, we have

$$\Delta_m'(P) = [P^2 + \mu_0^2 - g_0^2\Sigma(P^2)]^{-1}. \tag{6.5}$$

Therefore, the observed mass μ of the meson is given by

$$-\mu^2 + \mu_0^2 - g_0^2\Sigma(-\mu^2) = 0. \tag{6.6}$$

We eliminate μ_0 from (6.2) by the aid of (6.6). Then we have

$$F(q, P) = \frac{P^2 + \mu^2 + g_0^2\Sigma(-\mu^2)}{P^2 + \mu^2 - g_0^2[\Sigma(P^2) - \Sigma(-\mu^2)]} F_0(q, P). \tag{6.7}$$

From this we see that the mass of the deuteron m_d (we still refer to the compound particle of nucleon and antinucleon as the deuteron) is determined by

$$-m_d^2 + \mu^2 - g_0^2[\Sigma(-m_d^2) - \Sigma(-\mu^2)] = 0. \tag{6.8}$$

$f(q, D)$, which is defined as the residue of $F(q, P)$, now becomes, on account of (6.7) and (6.8),

$$f(q, D) = g_0^2\Sigma(-m_d^2)[1 - g_0^2\Sigma'(-m_d^2)]^{-1}F_0(q, D). \tag{6.9}$$

Inserting this into the normalization condition (1.8), and using (6.4), we have

$$|N|^{-2} = g_0^2\Sigma(-m_d^2)^2[1 - g_0^2\Sigma'(-m_d^2)]^{-1}. \tag{6.10}$$

Therefore it is necessary for the normalizability that

$$1 - g_0^2\Sigma'(-m_d^2) > 0. \tag{6.11}$$

When this condition is satisfied, the Bethe-Salpeter wavefunction defined by (1.5) becomes by the insertion of (6.9) and (6.10)

$$\chi(x_1, x_2; D) = -i(2\pi)^{-4}g_0[1 - g_0^2\Sigma'(-m_d^2)]^{-1/2} \times \int d^4q F_0(q, D) \times \exp[i(\tfrac{1}{2}D + q)x_1 + i(\tfrac{1}{2}D - q)x_2] \tag{6.12}$$

up to an undetermined phase factor.

$F_0(q, P)$ is the same as $F(q, P)$ which is given by (2.2). From (2.2) and (6.4) we see that $\Sigma(P^2)$ is a divergent quantity. But $\Sigma(P^2) - \Sigma(-\mu^2)$ and $\Sigma'(P^2)$ are found to be finite. Therefore, the eigenvalue equation (6.8) is meaningful, and the Bethe-Salpeter wavefunction remains finite in spite of divergency of the normalization integral.

Next we consider the deuteron-proton-antineutron vertex function

$$\bar{\Gamma}(-(D - \bar{n})^2) \equiv 2V(\bar{n}_0 D_0)^{1/2}\langle \bar{n} | j_\nu(0) | D\rangle, \tag{6.13}$$

where $|\bar{n}\rangle$ is the single antineutron state with the four-momentum $\bar{n}$. Equations (3.2), (3.3), and (3.4) still hold for this function. In (3.4), however, $f(q, D)$ is now given by (6.9). From (3.3), (3.4), (6.9), and (6.10) we have

$$\bar{\Gamma}(-(D - \bar{n})^2) = g_0[1 - g_0^2\Sigma'(-m_d^2)]^{-1/2}\bar{V}(\tfrac{1}{2}D - \bar{n}, D), \tag{6.14}$$

where

$$\bar{V}(q, P) \equiv [(\tfrac{1}{2}P + q)^2 + m^2] \times [(\tfrac{1}{2}P - q)^2 + m^2]F_0(q, P). \tag{6.15}$$

Using (2.2) for the expression of $F_0(q, P)$, we have in the same way as in the derivation of (3.6),

$$\bar{V}(q, P) = 1 + \lambda\int_{-1}^{1} dz \int_0^\infty dt \int_0^\infty dt' k_0(z, t; z, t'; P^2) \times [\xi_0(P^2)\,\delta(t') + \eta_0(z, t'; P^2)] \times t[q^2 + z(q\cdot P) + m^2 + P^2/4 + t]^{-1}. \tag{6.16}$$

Using this, we can rewrite (6.14) in the following form:

$$\bar{\Gamma}(x) = \Gamma_0 + \frac{1}{\pi}\int_{m^2}^\infty dx' \frac{\bar{\rho}(x')}{x' - x}, \tag{6.17}$$

where $\bar{\rho}(x')$ is given by an expression similar to (3.8). The constant Γ_0 comes from the first term in the right-hand side of (6.16). The renormalized deuteron-proton-antineutron coupling constant $\bar{\Gamma}_d$ is defined by $\bar{\Gamma}_d \equiv \bar{\Gamma}(m^2)$. Because of (6.14) it is proportional to $\bar{V}(q, P)$ in which all the four-momenta carried by the three particles are on the mass shell. On the other hand, when $(P/2 + q)^2 = (P/2 - q)^2 = -m^2$, the last two factors in the last term in (6.16) disappear, and as a result of (2.3) and (2.4) $\bar{V}(q, P)$ reduces to $\xi_0(P^2)$. Therefore we have from (6.14)

$$\bar{\Gamma}_d = g_0\xi_0(-m_d^2)[1 - g_0^2\Sigma'(-m_d^2)]^{-1/2}. \tag{6.18}$$

Finally we reconsider the above result from the viewpoint of renormalization theory. We first notice that (6.8) is symmetrical in μ and m_d. Therefore we can exchange the role of the deuteron with that of the physical meson, and apply the renormalization procedure regarding the deuteron as an elementary particle. Then we find that $\bar{V}(q, P)$ is the proper vertex part, and that its value on the mass shell $\xi_0(-m_d^2)$ is related to the renormalization constant Z_1 as

$$\xi_0(-m_d^2) = Z_1^{-1}. \tag{6.19}$$

On the other hand, if we rewrite (6.5) by the use of (6.6) as

$$\Delta_m'(P) = \{(P^2 + \mu^2)[1 - g_0^2\Sigma'(-\mu^2)] - g_0^2[\Sigma(P^2) - \Sigma(-\mu^2) - (P^2 + \mu^2)\Sigma'(-\mu^2)]\}^{-1},$$

and replace μ by m_d, we find that

$$1 - g_0^2\Sigma'(-m_d^2) = Z_3^{-1}. \tag{6.20}$$

Therefore (6.18) can be rewritten as

$$\bar{\Gamma}_d = g_0 Z_1^{-1} Z_3^{1/2}. \tag{6.21}$$

This is the same result as in the renormalization theory, because $Z_2 = 1$ in the present approximation. Because of (6.20), the normalizability condition (6.11) becomes $Z_3 > 0$, which is required in the renormalization theory. The renormalization theory also requires $Z_3 < 1$. It is interesting to see the implication of this restriction on our solution.

APPENDIX

From (2.5) and (2.8) we have

$$k_0^{(2)}(z, t; z', t'; P^2) = (4t)^{-1} \int_{-1}^{1} dz'' R(z'', z') \times \theta\{t\rho(z, z'') - \mu^2 - 2\mu[m^2 + (1 - z''^2)P^2/4]^{1/2}\} \times \int_{a+}^{b-} dt'' t''^{-1} A(t'')B(t'') \times [(b_+ - t'')(b_- - t'')(t'' - a_+)(t'' - a_-)]^{-1/2} \tag{A1}$$

with the abbreviations

$$A(t'') = [t'' - R(z'', z')(t' - \mu^2)] \times \{t'' + R(z'', z')[m^2 + (1 - z'^2)P^2/4]\}^{-1}$$

$$B(t'') = [t\rho(z, z'') - t'' + \mu^2] \times [t\rho(z, z'') + m^2 + (1 - z''^2)P^2/4]^{-1}$$

$$a_\pm = R(z'', z')\{t' + \mu^2 \pm 2\mu \times [t' + m^2 + (1 - z'^2)P^2/4]^{1/2}\}$$

$$b_\pm = t\rho(z, z'') + \mu^2 \pm 2\mu \times [t\rho(z, z'') + m^2 + (1 - z''^2)P^2/4]^{1/2}$$

$$R(z'', z') = 1/\rho(z'', z').$$

We assume that $-4m^2 \leq P^2 \leq 0$. Then we easily find that, in the integrand of (A1),

$$0 < t''^{-1} \leq a_+^{-1} < \{R(z'', z') \times [\mu^2 + 2\mu(m^2 + P^2/4)]\}^{-1}$$

$$0 < A(t'') < 2$$

$$0 < B(t'') < (\mu^2 + m^2 + P^2/4)(m^2 + P^2/4)^{-1}$$

$$0 < (t'' - a_-)^{-1/2} \leq (a_+ - a_-)^{-1/2} \leq \tfrac{1}{2}[\mu R(z'', z')(m^2 + P^2/4)^{1/2}]^{-1/2}$$

$$0 < (b_+ - t'')^{-1/2} \leq (b_+ - b_-)^{-1/2} \leq \tfrac{1}{2}\mu^{-1/2} t^{-1/4} \rho(z, z'')^{-1/4}$$

$$0 \leq \theta\{t\rho(z, z'') - \mu^2 - 2\mu[m^2 + (1 - z''^2)P^2/4]^{1/2}\} \leq \theta\{4t(1 - z^2)^{-1} - \mu^2 - 2\mu(m^2 + P^2/4)^{1/2}\}.$$

In obtaining the last inequality we have used $\rho(z, z'') \leq 4(1 - z^2)^{-1}$. From (A1) and the above inequalities we have

$$0 \leq k_0^{(2)}(z, t; z', t'; P^2) < (8\mu)^{-1}(\mu^2 + m^2 + P^2/4) \times (m^2 + P^2/4)^{-5/4}[\mu^2 + 2\mu(m^2 + P^2/4)^{1/2}]^{-1} t^{-5/4} \times \theta[4t(1 - z^2)^{-1} - \mu^2 - 2\mu(m^2 + P^2/4)^{1/2}] \times \int_{-1}^{1} dz'' \rho(z, z'')^{-1/4} \times \rho(z'', z')^{1/2} \int_{a+}^{b-} dt''(b_- - t'')^{-1/2}(t'' - a_+)^{-1/2}. \tag{A2}$$

The last integral over t'' merely reduces to π. From (A2) and (2.9) we have

$$0 \leq [\partial\tau(z, \sigma)/\partial\sigma] k_0^{(2)}(z, \tau(z, \sigma); z', \tau(z', \sigma'); P^2) < (\pi/\sqrt{2})(\mu^2 + m^2 + P^2/4) \times m^{-1/2}\mu^{-1}(m^2 + P^2/4)^{-5/4} \times [\mu^2 + 2\mu(m^2 + P^2/4)^{1/2}]^{-1} \times \theta\{\sigma - [\mu^2 + 2\mu(m^2 + P^2/4)^{1/2}] \times [m^{1/2} + [\mu^2 + 2\mu(m^2 + P^2/4)^{1/2}]^{1/4}]^{-1}\}\sigma^{-2} \times (1 - z^2)^{-1/4} \int_{-1}^{1} dz'' \rho(z, z'')^{-1/4} \rho(z'', z')^{1/2}. \tag{A3}$$

But it is easily proved that

$$(1 - z^2)^{-1/4} \int_{-1}^{1} dz'' \rho(z, z'')^{-1/4} \rho(z'', z')^{1/2} < 11(2)^{1/2}. \tag{A4}$$

From (A3) and (A4) follows (2.10).

A Summation Procedure for Certain Feynman Integrals*

DONALD G. BABBITT
Aerospace Corporation, El Segundo, California,
and
Department of Mathematics, University of California, Los Angeles, California
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A mathematically rigorous summation procedure is developed for Feynman integrals involving a repulsive potential. The central idea of the proof is to connect certain Wiener integrals with the Feynman integral in question by making use of holomorphic vector-valued functions and holomorphic semigroups.

INTRODUCTION

An approach to nonrelativistic quantum mechanics based on the classical Lagrangian of the system in question and an action principle has been formulated by Feynman.[1] In particular, for a system whose classical behavior is governed by a scalar potential $V(x)$, $x \in E^m$, he was able, after several formal simplifications, to write the quantum mechanical evolution of the system with initial state $\psi(x)$, $\int_{E^m} |\psi|^2\, dx < \infty$, as follows:

$$\psi(x, t) = \lim_{n\to\infty} \left(\frac{2\pi i t}{n}\right)^{-mn/2} \int_{E^m} \cdots \int_{E^m} \psi(x_0) \times \prod_1^n \left\{ \exp i\left[\frac{(x_i - x_{i-1})^2}{2t/n} - \frac{t}{n} V(x_{i-1})\right]\right\} \times dx_0 \cdots dx_{n-1}, \quad (1)$$

where $x_n = x$ and where we have assumed, for simplicity, that $\hbar = 1$ and mass is equal to 1. Feynman then formally showed that Eq. (1) was the solution of the Schrödinger equation for the system.

Since Feynman's arguments were purely formal, one might ask, What is the precise mathematical meaning of the "limit" appearing in Eq. (1) and when does the "limit" satisfy Schrödinger's equation and in what sense? It is to these questions that we address ourselves in this paper.

If one replaces the term it by t in Eq. (1), one can apply the theory of the Wiener integral and conclude that the limit exists pointwise and is a solution of the heat equation with perturbation $-V(x)$. It was thus hoped a similar complex measure was underlying the Feynman integral; i.e., Eq. (1). This does not appear to be the case.[2,3] Thus, we seem to be left with interpreting Eq. (1) as a problem of sequences and not, unfortunately, as the limit of Riemann approximations to the integral of a continuous function over "Feynman" space.

We will proceed as follows: In Theorem I, we replace i by $-1/\sigma$, Re $(\sigma) > 0$, in the integrals appearing in Eq. (1); we then take the L_2 limit, which exists for a large class of $V(x)$, and finally we let $\sigma \to \pm i$ in L_2. The double limit defines a unitary flow of $\psi(x)$. We are able to characterize the infinitesimal generator of the flow in terms of the Wiener integral which, in most cases, implies the double limit is a solution of Schrödinger's equation. Theorem II and the corollary show that the above limiting process is a valid summation procedure.

NOTATION

The term E^m will denote the space of real m-tuples. Elements in E^m will be denoted by x or y, with or without subscripts, and for

$$x = (x^1 \cdots x^m), \quad |x| = [(x^1)^2 + \cdots + (x^m)^2]^{1/2}.$$

The term $L_2(E^m)$ will denote the vector space of complex-valued, Lebesgue square-summable functions modulo the space of null functions. For $\psi(x)$ and $\phi(x)$ in $L_2(E^m)$, let $(\psi, \phi) = \int \bar{\psi}\phi\, dx$ and $||\psi||^2 = (\psi, \psi)$. With this norm, $L_2(E^m)$ is a complex Hilbert space. We say ψ_n converges to ψ in L_2 if $||\psi_n - \psi|| \to 0$ as $n \to \infty$. We also say l.i.m.$_{n\to\infty}$ $\psi_n(x) = \psi(x)$. If A is a bounded linear operator on $L_2(E^m)$,

$$||A||_{op} = \sup_{||\psi||=1} ||A\psi||.$$

If A is an unbounded operator on $L_2(E^m)$, $\mathfrak{D}(A)$ will denote the domain of A. The term I will denote the identity operator on $L_2(E^m)$.

R^+ will denote the complex numbers with positive real part. Since we make extensive use of the complex Gaussian kernel in E^m, we will use a special notation for it; i.e., for x in E^m, z in R^+, let

$$p(x, z) = (2\pi z)^{-m/2} \exp[-|x|^2/2z].$$

* This paper is essentially a portion of the author's thesis written under the guidance of Professor D. A. Darling at the University of Michigan.

[1] R. P. Feynman, Revs. Modern Phys. **20**, 367 (1948).

[2] R. H. Cameron, J. Math. and Phys. **39**, 126 (1960).

[3] I. M. Gelfand and A. M. Yaglom, J. Math. Phys. **1**, 48 (1960).

It is well known that $p(x, t)$, $t > 0$, can be used to define a countably additive measure (Wiener measure) on the space C_t of continuous functions from $[0, t]$ to E^m which vanish at 0. If $F_t(\cdot)$ is a summable functional on this probability space, then its expectation will be denoted by $E\{F_t[x(\ )]\}$. This quantity is also known as the Wiener integral[4] of the functional $F_t(\cdot)$. The term Δ will denote the Laplacian in E^m. In our proofs we will make use of the theory of strongly continuous semigroups of operators on $[0, \infty)$, Hilbert-space and operator-valued holomorphic functions and holomorphic semigroup of operators. Hille and Phillips[5] have given their precise definition and main properties.

STATEMENT OF THEOREMS

Theorem I

Let $V(x)$ be a real-valued continuous function on E^m which is bounded on bounded sets and bounded below everywhere by $M > -\infty$. For $\psi(x) \in L_2(E^m)$ and $z \in R^+$, define

$$(T_n(z)\psi)(x) \equiv \int_{E^m} \cdots \int_{E^m} \psi(x_0) \times \prod_{j=1}^{n} \left\{ p\left(x_j - x_{j-1}, \frac{z}{n}\right) \exp\left[-\frac{z}{n} V(x_{j-1}) \right] \right\} \times dx_0 \cdots dx_{n-1},$$

where $x_n \equiv x$. Then $(T_n(z)\psi)(x) \equiv T_n(z)\psi$ is in $L_2(E^m)$ and for $\sigma \in R^+$ and $t > 0$

$$\underset{\sigma \to i}{\text{l.i.m.}} \left[\underset{n \to \infty}{\text{l.i.m.}} T_n(\sigma t)\psi \right] \tag{2}$$

and

$$\underset{\sigma \to -i}{\text{l.i.m.}} \left[\underset{n \to \infty}{\text{l.i.m.}} T_n(\sigma t)\psi \right] \tag{3}$$

exists and equals $U_{\pm t}\psi \equiv \psi(x, \pm t)$, where U_t, $-\infty < t < \infty$ is a continuous unitary group of operators on $L_2(E^m)$. In fact, if we denote the infinitesimal generator of U_t by iA, then A is the infinitesimal generator of the strongly continuous, self-adjoint semigroup of operators $T(t)$, which is defined as follows:

$$T(t)\psi \equiv E\left\{ \exp\left[-\int_0^t V(x(\tau) + x)\, d\tau \right] \psi(x(\tau) + x) \right\}$$

for $t > 0$ and $\psi \in L_2(E^m)$.

[4] For definitions and details, see M. Kac, *Probability and Related Topics in the Physical Sciences: Lectures in Applied Mathematics* (Interscience Publishers, Inc., New York, 1959), Vol. 1, Chap. 4.

[5] E. Hille and R. S. Phillips, Colloq. Publications Am. Math. Soc., **31** (1957).

Remark 1. From the general theory of semigroups, we know that for $\psi \in \mathfrak{D}(A)$, $\psi(x, t)$ satisfies

$$\partial\psi/\partial t = (iA)\psi(x, t)$$

and

$$||\psi(x, t) - \psi(x)|| \to 0$$

as $t \to 0$. By $\partial\psi/\partial t$ we mean the L_2 derivative of $\psi(x, t)$ with respect to t.

The above remark shows that Eqs. (2) and (3) define the solution of Schrödinger's equation with initial state $\psi(x)$ if $\psi \in \mathfrak{D}(A)$ and $A = \frac{1}{2}\Delta - V(x)$. This, in fact, is the case when $V(x)$ satisfies certain mild smoothness conditions.[6]

Theorem II

Suppose the same definitions and hypotheses hold as in Theorem I. If

$$\underset{n \to \infty}{\text{l.i.m.}} \left[\underset{\sigma \to i}{\text{l.i.m.}} T_n(\sigma t)\psi \right] \equiv \underset{n \to \infty}{\text{l.i.m.}} \left[T_n(it)\psi \right] \tag{4}$$

exists and is weakly continuous in t, then this limit equals $U_t\psi$. A similar argument holds for $\sigma \to -i$.

Corollary. Let the matrix $B = (b_{kj})$, $k = 1, 2 \cdots$, $j = 1, 2 \cdots$, define a regular method of summability for Hilbert space-valued sequences.[7]

If, for $t > 0$ and $\psi \in L_2(E^m)$,

$$T_n(it)\psi \equiv \underset{\sigma \to i}{\text{l.i.m.}} T_n(\sigma t)\psi$$

is B summable to a weakly continuous function of t, then this limit is equal to $U_t\psi$. A similar argument holds for $\sigma \to -i$.

Remark 2. Theorems I and II show that the double limits of Eqs. (2) and (3) can be used as a valid summation procedure for the sequence $T_n(it)\psi$.

PROOF OF THEOREM I

We shall give details of the proof of this theorem, Theorem II, and the corollary for the case $V(x) \geq 0$. The extension of the arguments to the general case where $V(x) \geq M > -\infty$ will be obvious.

For $z \in R^+$, $\psi(x) \in L_2(E^m)$, define

$$\left(\tilde{T}_1(z)\psi \right)(x) \equiv \int_{E^m} p(x - x_1)\psi(x_1) \right) dx_1.$$

It is known[8] that $\tilde{T}_1(z)$ is a holomorphic semigroup

[6] D. Ray, Trans. Am. Math. Soc. **71**, 120 (1951).

[7] See exercises 34-36 on pages 74 and 75 of this reference N. Dunford and J. Schwartz, *Linear Operators, Part I* (Interscience Publishers Inc., New York, 1958) for definitions and properties. Dunford and Schwartz only consider complex-valued sequences, but the extension to Hilbert space-valued sequences is obvious.

[8] Reference 5, pages 602 and 603.

in R^+ such that $||\tilde{T}_1(z)||_{op} \leq 1$ and that $\tilde{T}_1(t)$, $t > 0$, is a strongly continuous self-adjoint semigroup on $(0, \infty)$ such that $\lim_{t\to 0} \tilde{T}_1(t) = I$ in the strong operator topology. It follows from the general theory[9] that

$$\text{l.i.m.}_{\sigma\to i} \tilde{T}_1(\sigma t),$$

$$\text{l.i.m.}_{\sigma\to -i} \tilde{T}_1(\sigma t)$$

exists for $t > 0$, $\sigma \in R^+$ and $\psi \in L_2(E^m)$ and moreover defines a strongly continuous unitary group $\tilde{T}_1(it)$, $-\infty < t < \infty$.

Also for $z \in R^+$, $\psi(x) \in L_2(E^m)$, define

$$\tilde{T}_2(z)\psi \equiv \{\exp[-zV(x)]\}\psi(x).$$

It is clear that $\tilde{T}_2(z)$ defines a holomorphic semigroup on R^+ such that $||\tilde{T}_2(z)||_{op} \leq 1$.[10] Moreover $\tilde{T}_2(t)$ is easily defined on $[0, \infty]$ and is a strongly continuous self-adjoint semigroup there. For the reasons mentioned above (or by direct proof)

$$\text{l.i.m.}_{\sigma\to i} \tilde{T}_2(\sigma t)\psi,$$

$$\text{l.i.m.}_{\sigma\to -i} \tilde{T}_2(\sigma t)\psi$$

exist for $t > 0$, $\sigma \in R^+$ and $\psi \in L_2(E^m)$ and defines a strongly continuous unitary group $\tilde{T}_2(it)$, $-\infty < t < \infty$.

With these definitions of $\tilde{T}_1(z)$ and $\tilde{T}_2(z)$, we see that

$$T_n(z)\psi = [\tilde{T}_1(z)\tilde{T}_2(z)]^n\psi$$

for $z \in R^+$, $\psi \in L_2(E^m)$. Since $\tilde{T}_1(z)$ and $\tilde{T}_2(z)$ are bounded operators on $L_2(E^m)$, it is clear that $T_n(z)\psi$ is in $L_2(E^m)$; in fact,

$$||T_n(z)\psi|| \leq ||\psi||.$$

$T_n(z)\psi$ has two other properties which will be of use to us later. The first is that $T_n(z)\psi$ is holomorphic in R^+. This follows from the holomorphy of $\tilde{T}_1(z)$ and $\tilde{T}_2(z)$ and the fact that products of holomorphic operator-valued functions are holomorphic. The second property is that

$$\text{l.i.m.}_{\sigma\to i} T_n(\sigma t)\psi = \left[\tilde{T}_1\left(\frac{it}{n}\right)\tilde{T}_2\left(\frac{it}{n}\right)\right]^n\psi,$$

$$\text{l.i.m.}_{\sigma\to -i} T_n(\sigma t)\psi = \left[\tilde{T}_1\left(-\frac{it}{n}\right)\tilde{T}_2\left(-\frac{it}{n}\right)\right]^n\psi$$

for $\sigma \in R^+$, $t > 0$ and $\psi(x) \in L_2(E^m)$. This follows directly from the properties of $\tilde{T}_j(z)$, $j = 1, 2$, and the fact that multiplication is continuous in the strong operator topology providing the multiplicands are uniformly bounded.

To complete the proof we will need the following two lemmas.

Lemma I. If $t > 0$, $\psi(x) \in L_2(E^m)$ and $V(x)$ as in Theorem I, then[11]

$$\lim_{n\to\infty} \int_{E^m} \cdots \int_{E^m} \psi(x_0) \prod_{j=1}^{n} \{p(x_j - x_{j-1})t \times \exp[-(t/n)V(x_{j-1})]\}\, dx_0 \cdots dx_{n-1} = E\left\{\exp\left[-\int_0^t V(x(\tau) + x)\, d\tau\right]\psi(x(t) + x)\right\}. \quad (5)$$

The proof for the above hypotheses is as follows:

$$\exp\left[\left(\frac{kt}{n}\right)\sum_{k=1}^{n} V\left(x\left(\frac{kt}{n}\right) + x\right)\right]\psi(x(t) + x)$$

is a measureable functional on C_t with respect to Wiener measure. Moreover, for $x(\tau) \in C_t$,

$$\lim_{n\to\infty} \exp\left[-\frac{t}{n}\sum_{k=1}^{n} V\left(x\left(\frac{kt}{n}\right) + x\right)\right]\psi(x(t) + x) = \exp\left[-\int_0^t V(x(\tau) + x)\, d\tau\right]\psi(x(t) + x).$$

Thus, since

$$\left|\exp\left[-\frac{t}{n}\sum_{k=1}^{n} V\left(x\left(\frac{kt}{n}\right) + x\right)\right]\psi(x(t) + x)\right| \leq |\psi(x(t) + x)|$$

and $\psi(x(t) + x)$ is integrable with respect to Wiener measure on C_t, we can apply the abstract dominated convergence theorem and conclude that

$$\lim_{n\to\infty} E\left\{\exp\left[-\frac{t}{n}\sum_{k=1}^{n} V\left(x\left(\frac{kt}{n}\right) + x\right)\right]\psi(x(t) + x)\right\} = E\left\{\exp\left[-\int_0^t V(x(\tau) + x)\, d\tau\right]\psi(x(t) + x)\right\}.$$

But,

$$E\left\{\exp\left[-\frac{t}{n}\cdot\sum_{k=1}^{n} V\left(x\left(\frac{kt}{n}\right) + x\right)\right]\psi(x(t) + x)\right\} = \int_{E^m} \cdots \int_{E^m} \prod_{1}^{n} \{p(x_j - x_{j-1}) \times \exp[-(t/n)V(x_j + x)]\} \times \psi(x_n + x)\, dx_0 \cdots dx_{n-1}, \quad (6)$$

where $x_0 = 0$, and when we make the change of variables $x_j = y_{n-j}$, $j = 1, 2, \cdots n$, in Eq. (6) we see that Eq. (5) follows:

[9] Reference 5, Theorem 17.9.1-2.

[10] Here is an example of where, in the general case, we would replace 1 in the above equality by $\exp[-|M|\,\mathrm{Re}(z)]$.

[11] lim here means the pointwise limit.

Lemma II. Let us assume the same hypotheses hold as in Lemma I. Then

$$\text{l.i.m.}_{n\to\infty} T_n(t)\psi = T(t)\psi, \tag{7}$$

where $T(t)$ is defined in Theorem I.

The proof for Lemma II is as follows: Since $||T_n(t)|| \leq 1$, it will be sufficient to show that Eq. (7) is true for functions $\psi \in C_\infty(E^m)$,[12] by the uniform boundedness theorem. We can reduce the problem further by noting $||T_n(t)\psi|| \leq ||\psi||$, $\psi \in C_\infty(E^m)$, and thus, by applying standard Hilbert space theory and the uniform boundedness theorem again, we have

$$\text{l.i.m.}_{n\to\infty} T_n(t)\psi = T(t)\psi, \qquad \psi \in C_\infty(E^m)$$

if, and only if,

$$\text{(a)} \quad \lim_{n\to\infty} ||T_n(t)\psi||^2 = ||T(t)\psi||^2, \quad \psi \in C_\infty(E^m)$$
$$\text{(b)} \quad \lim_{n\to\infty} (T_n(t)\psi, \phi) = (T(t)\psi, \phi), \quad \psi, \phi \in C_\infty(E^m). \tag{8}$$

Since

$$|(T_n(t)\psi)(x)| \leq \int_{E^m} p(x-y)\,|\psi(y)| = \Lambda(x) \in L_2(E^m)$$

for $\psi \in C_\infty(E^m)$, and, therefore,[13]

$$|(T_n(t)\psi)(x)|^2 \leq |\Lambda(x)|^2 \in L_1(E^m),$$

and using Lemma I, we can apply the abstract dominated convergence theorem and conclude

$$\lim_{n\to\infty} ||T_n(t)\psi||^2 = \lim_{n\to\infty} \int_{E^m} |(T_n(t)\psi)(x)|^2\,dx$$
$$= \int_{E^m} \lim_{n\to\infty} |(T_n(t)\psi)(x)|^2\,dx$$
$$= \int_{E^m} |(T(t)\psi)(x)|^2\,dx = ||T(t)\psi||^2.$$

Thus condition (a) is proved.

To prove condition (b), note:

$$\overline{|(T_n(t)\psi)(x)}\phi(x)|$$
$$\leq K \int_{E^m} p(x-y,t)\,|\psi(y)|\,dy \equiv \xi(x)$$

where $K = \max_{x\in E^m} |\phi(x)|$. $\xi(x)$ is in $L_1(E^m)$ since $|\psi(y)| \in L_1(E^m)$ and $p(x,t)$ defines a map of L_1 into L_1 by convolution. Thus, applying Lemma I and the dominated convergence theorem, we conclude

$$\lim_{n\to\infty} (T_n(t)\psi, \phi) = \lim \int_{E^m} \overline{(T_n(t)\psi)(x)}\phi(x)\,dx$$
$$= \int_{E^m} \lim \overline{(T_n(t)\psi)(x)}\phi(x)\,dx = \int_{E^m} \overline{(T(t)\psi)(x)}\phi(x)$$
$$= (T(t)\psi, \phi).$$

Thus, in lieu of the equivalence of Eqs. (7) and (8), the lemma is proved.

Completing the proof of Theorem I, we know[14] that $T(t)$ is a strongly-continuous, self-adjoint semigroup of operators on $[0, \infty)$. We shall denote its self-adjoint infinitesimal generator by A. Moreover, by the above remarks, we have, for each $\psi \in L_2(E^m)$, a sequence of vector-valued functions $T_n(z)\psi$ such that

(i) $T_n(z)\psi$ is holomorphic in R^+ for $n = 1, 2 \cdots$
(ii) $||T_n(z)\psi|| \leq ||\psi||$
(iii) for $t > 0$, $\text{l.i.m.}_{n\to\infty} T_n(t)\psi = T(t)\psi$.

Thus we can apply Vitali's theorem[15] and conclude

$$\text{l.i.m.}_{n\to\infty} T_n(z)\psi = T(z)\psi$$

for $z \in R^+$ and $T(z)\psi$ is a holomorphic vector-valued function in R^+ such that $||T(z)\psi|| \leq ||\psi||$. Since this is true for each $\psi \in L_2(E^m)$, $T(z)$ is a holomorphic operator-valued function which is an extension of $T(t)$ to R^+. In fact $T(z)$ is a holomorphic semigroup. This follows from the general theory[16] or by direct verification.

In new notation, Eq. (9) says

$$\text{l.i.m.}_{n\to\infty} T_n(\sigma t)\psi = T(\sigma t)\psi \tag{9a}$$

for $\sigma \in R^+$, $t > 0$. From the general theory[17] we can thus conclude

$$\text{l.i.m.}_{\sigma\to i} T_n(\sigma t)\psi = T(it)\psi$$
$$\text{l.i.m.}_{\sigma\to -i} T_n(\sigma t)\psi = T(-it)\psi, \tag{10}$$

where $T(it)$, $-\infty < t < \infty$, is a strongly continuous group of operators with infinitesimal generator iA. Since A is self-adjoint, $T(it) \equiv U_t$ is a unitary group by Stone's theorem. Since Eq. (10), in lieu of (9a), is exactly Eqs. (2) and (3), Theorem I is proved.

PROOF OF THEOREM II

For an arbitrary pair ψ and χ in $L_2(E^m)$, let

$$\phi_k(z) = (T_k(z)\psi, \chi), \qquad k = 1, 2 \cdots.$$

[12] $C_\infty(E^m)$ = space of (complex) continuous functions on E^m with compact support.
[13] Where $L_1(E^m) = \{\psi \mid \int_{E^m} |\psi|\,dx < \infty\}$.
[14] Reference 6.
[15] Reference 5, Theorem 3.14.1.
[16] Reference 5, Theorem 17.2.1.
[17] Reference 5, Theorem 17.9.1–2.

The terms $\phi_k(z)$ are analytic functions in R^+, bounded by $||\psi||\ ||\chi||$. These properties follow from the discussion of the $T_k(z)$ given in the proof of Theorem I. Moreover, by the hypothesis of the theorem,

$$\lim_{k\to\infty}[\lim_{z\to it}\phi_k(z)] \equiv \lim_{k\to\infty}[\phi_k(it)] \equiv (W(t)\psi, \chi)$$

exists and is continuous for $-\infty < t < \infty$. With conformal mapping we can apply the theorem of Ostrowski and Khinchin[18] and conclude

$$\lim_{k\to\infty}\phi_k(z) = (T(z)\psi, \chi)$$

for $z \in R^+$, and, thus, for $t > 0$,

$$\begin{aligned}\lim_{z\to it}(T(z)\psi, \chi) &\equiv (U_t\psi, \chi) = (W(t)\psi, \chi)\\ \lim_{z\to -it}(T(z)\psi, \chi) &\equiv (U_{-t}\psi, \chi) = (W(-t)\psi, \chi)\end{aligned} \tag{11}$$

almost everywhere. But since the last two terms in each expression of Eq. (11) are continuous, they must be equal everywhere. Since χ was arbitrary, $U_t\psi = W(t)\psi$, which proves Theorem II.

PROOF OF THE COROLLARY

The corollary will be proved by the same reasoning as Theorem II if we can show:

$$\text{l.i.m.}_{k\to\infty}\sum_{j=1}^{\infty} b_{kj}T_j(z)\psi = T(z)\psi \tag{12}$$

for $z \in R^+$, and

$$\text{l.i.m.}_{z\to it}\sum_{j=1}^{\infty} b_{kj}T_j(z)\psi = \sum_{j=1}^{\infty} b_{kj}T_j(it)\psi, \tag{13}$$

and similarly for $z \to -it$.

Since $\text{l.i.m.}_{k\to\infty}\ T_k(z)\psi = T(z)\psi$, $z \in R^+$, the Silverman-Toeplitz theorem[7] applies and Eq. (12) is proved.

To prove Eq. (13), note that

$$\begin{aligned}\left|\left|\sum_{j=1}^{\infty} b_{kj}[T_j(z) - T_j(it)]\psi\right|\right| &\le \sum_{j=1}^{\infty}|b_{kj}|\ ||T_j(z)\psi - T_j(it)\psi||\\ &\le \sum_{j=1}^{J}|b_{kj}|\ ||T_j(z)\psi - T_j(it)\psi||\\ &\quad + 2\sum_{j=J+1}^{\infty}|b_{kj}|\ ||\psi||.\end{aligned}$$

For $\epsilon > 0$ and $J(\epsilon) = J$ sufficiently large, the above is less than or equal to

$$\sum_{j=1}^{J}|b_{kj}|\ ||T_j(z)\psi - T_j(it)\psi|| + 2\epsilon\ ||\psi||,$$

and for z sufficiently close to it,

$$||T_j(z)\psi - T_j(it)\psi|| \le \epsilon/J, \qquad j = 1, 2 \cdots J,$$

and hence

$$\left|\left|\sum_{j=1}^{\infty} b_{kj}[T_j(z)\psi - T_j(it)\psi]\right|\right| \le \epsilon + 2\epsilon\ ||\psi||.$$

The same reasoning applies when z is sufficiently close to the term $-it$, and, thus, Eq. (13) is proved and the corollary is proved.

CONCLUDING REMARKS

Remark 3. In lieu of the preceding theorems, we make the following definition: Let $V(x)$ and $\psi(x)$ be as in Theorem I, then the "sequential" Feynman integral[19] of the functional

$$\exp\left[i\int_0^{t'}\left\{\left(\frac{dx}{d\tau}\right)^2 - V(x(\tau))\right\}d\tau\right]\psi(x(0))$$

is defined by Eq. (2) if $t' = t > 0$ or by Eq. (3) if $t' = -t$, $t > 0$. It is often denoted by

$$N^{-1}\int\cdots\int\psi(x(0))\exp\left[i\int_0^{t'}\left\{\left(\frac{dx}{d\tau}\right)^2 - V(x(\tau))\right\}d\tau\right]\prod_{0\le\tau<t'}dx(\tau),$$

where N is a singular normalizing constant.

We might also have defined the integral as the boundary value of the analytic extension to R^+ of the Wiener integral, Eq. (9), at (it).

Remark 4. It was merely a matter of convenience that we partitioned the interval $[0, t]$ into n equal parts. We might just as well have used a sequence Δ_n of partitions of $[0, t]$ where the mesh of Δ_n goes to 0 as n goes to ∞.

Remark 5. The techniques used in the proofs of Theorems I and II generalize directly to cover (a) the case where $V(x) = +\infty$ outside a reasonably smooth region Ω in E^m, and (b) the case where V depends explicitly on t, providing certain properties hold for $V(x, t)$, uniformly for bounded intervals of t.

Most of the essential new results needed to prove Theorems I and II for case (a) are already included in Ray's paper.[7] For (b) one only needs an elementary theory of generalized semigroups similar to the theory we used from semigroups. Details of these generalizations will be given in a later paper.

[18] L. P. Priwalow, *Randeigenschaften Analytischer Functionen* (Deutscher Verlag der Wissenschaften, 1958), Theorem 7.1.

[19] This terminology was introduced by R. H. Cameron.

ADDENDUM

Since the completion of this paper, Professor Edward Nelson has brought to the attention of the author the fact that one can combine some results of Trotter[20] and Kato[21] and prove the limit Eq. (4) exists, and is weakly continuous, for a large class of interesting $V(x)$, $x \in E^m$. Our answer agrees by Theorem II; however the combined Trotter-Kato results do not seem to apply to the cases mentioned in remark 5.

[20] H. F. Trotter, Proc. Am. Math. Soc. **10**, 545 (1959).
[21] T. Kato, Trans. Am. Math. Soc. **70**, 196 (1951).

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A Unified Variational Formulation of Classical and Quantum Dynamics. I

EDWARD M. CORSON
Georgetown University, Washington, D. C.
(Received 17 August 1962)

We have critically re-examined the role and status of Lagrangian concepts in both classical and quantal contexts. We find a new, unified variational principle which, subject to the superadded postulates of *determinism* or *indeterminism*, respectively, leads uniquely to the classical concept of state and Lagrange equations of motion or to the quantal concept of state and Schrödinger equations of motion.

INTRODUCTION

IN the classical context, we critically re-examine the basic approach to physical theory and, in particular, the role and status of the Hamiltonian principle of stationary action. It is well known that, via Newton's equations, generalized coordinates, and virtual displacements, the Lagrange equations are, indeed, conceptually primary. Subject to the obvious condition that essential classical relations are not violated, we remark that the usual action is *not at all unique* as the variation functional chosen as dynamical characteristic of the evolution of physical processes (determination of the concept of state and equations of motion—in the widest sense). Indeed, for the condition of stationarity which is all that is dynamically required, one has unlimited choice of possible functionals $F(S)$, from which the usual stationarity condition, $\delta S = 0$, follows. In particular, considering the evolution of a classical path from a somewhat unusual probabilistic point of view, we introduce as dynamical characteristic, the action phase functional exp $(iS/\hbar)$. This may be interpreted as probability amplitude, transition amplitude, or amplitude for arrival, between any two points of the classical path[1] and in either of two ways such that the usual action principle is either uniquely implied or tautologous [cf. Eqs. (1) and (1′) below].

In the quantal context, too, we cannot, and need not, avoid all the physical and mathematical developments of previous theory, in particular, the considerations of Dirac[2] pointing out an essential connection between coordinate-representation transformation amplitudes and Lagrangian concepts, and Feynman's[3] further extension of these basic ideas in the path-integral space-time approach. However, Dirac's basic considerations did not provide any well-defined, conclusive transition from quantal to classical formulations of the concept of state and corresponding equations of motion, or really explain the radically different roles and functional forms of the action in the two theories. Similarly, Feynman's considerations depend critically on starting from explicit prior knowledge of the Schrödinger equations, as well as quantal probabilistic concepts, and again do not explain the seemingly strange occurrence and form of the classical action in an essentially quantal context. Thus, despite their elegance and importance, these prior and basic investigations remain a somewhat unresolved combination of quantal and classical concepts and methods. Furthermore, contrary to the implications of most of the literature since Feynman's first article, they do not constitute an independent Lagrangian formulation of quantum dynamics as distinguished from the familiar Hamiltonian formulation. Moreover, there are many reasons that lead us to expect that a true Lagrangian formulation, in both contexts, should result from some simple variation principle.

As anticipated implicitly in the two preceding paragraphs, we synthesize these previous analyses as well as recast classical theory to formulate a single variation principle on a single characteristic functional such that:

(a) Subject to the added postulate of determinism (determinate path or history) we obtain the classical state and Lagrange equations of motion, and

(b) Subject to the alternate extreme postulate of indeterminism (indeterminate path or history) we obtain the corresponding quantal state and

[1] L. Motz [Phys. Rev. **126**, 378 (1962)], starting from entirely different and independent considerations of the Hamilton-Jacobi formalism, also finds this action phase functional appearing in an unique role in that it permits him to obtain the Hamiltonian operator corresponding to a given Hamilton-Jacobi equation by essentially algebraic manipulations. His procedure also leads to the path-integral formalism and affords one of the more direct of several alternative ways of going over from Lagrangian to Hamiltonian quantum formalism.

[2] P. A. M. Dirac, *Quantum Mechanics* (Oxford University Press, New York, 1957), 4th Ed., p. 125.

[3] R. P. Feynman, Revs. Modern Phys. **20**, 367 (1948); Phys. Rev. **80**, 440 (1950).

Schrödinger equations of motion. Thus, we show that there exists a single unifying dynamical principle from which both the classical and quantum theories emerge in Lagrangian form, diverging *solely* because of the superadded, respective postulates of determinism vs indeterminism. This seems to us to afford a significant insight into the space-time implications of determinism vs indeterminism as well as implying (one might even say proving) the necessity of the basic commutators, transformation theory, and all the familiar consequences in the alternate Hamiltonian formulation.[4]

BASIC POSTULATES AND EQUATIONS

Let us now express in condensed mathematical form, the essential steps corresponding to the preceding discussion, in the nonrelativistic domain. We consider the evolution of some physical system (the number of configuration space dimensions is irrelevant) from a given point in configuration space P_0, to a definite, but arbitrary, point P, and consider all possible continuous paths from P_0 to P. It does not matter, here, whether we follow the evolution of the system into past or future. We recognize that Hamilton's principle, $\delta S = 0$, $S = \int_{t_0}^{t} L\, d\tau$, *is entirely arbitrary*, since there are an infinite number of functions of S whose first variation implies $\delta S = 0$ (necessary and sufficient *but not unique*). In other words, the Hamiltonian principle is simply and *ex post facto* the most obvious form involving the invariant S that leads to Euler equations identical with the Lagrange equations, *but* the dynamical processes and equations are indifferent to the character of the extremum; only stationarity is required.

Now, to any path, geometrically considered, between P_0 and P, we assign the phase characteristic $\exp(iS/\hbar)$.

We take as our sole variational postulate I:

$$\delta \sum_{p \in C} \exp(iS_p/\hbar) = 0 \tag{1}$$

where $p \in C$ denotes the set of paths contained in the class of paths considered. There are, then, two obvious extreme cases:

(a) *Classical* (deterministic or definite path case)

$$\delta \exp(iS/\hbar) = 0. \tag{2a}$$

Here, $\delta S = 0$ is implied; the usual basic classical concept of state and equations of motion are an automatic consequence.

(b) *Quantal* (indeterministic or indefinite path case)

$$\delta \sum_{p} \exp(iS_p/\hbar) = \delta \int_{-\infty}^{\infty} \cdots \int \exp\left(\frac{i}{\hbar}\int_{t_0}^{t} L[x(\tau)]\, d\tau\right) \times \prod_{t_0}^{t} dx(\tau) = 0. \tag{2b}$$

Here, since all paths, including all possible variations, are already included in $\sum_p \exp(iS_p/\hbar)$, it follows that the latter is not a functional of path but merely a function of the fixed endpoints x, t; x_0, t_0, so that the variation is necessarily identically zero. Thus we find

$$\int \cdots \int \exp(iS[x]/\hbar) \prod_{t_0}^{t} dx(\tau) \equiv NK(x, t; x_0, t_0) \equiv N\langle x, t \mid x_0, t_0\rangle \tag{3}$$

where N is a constant. Here, we know that the left-hand side of Eq. (3) satisfies the Schrödinger equation for the transition amplitude (or Green's function)[5]; the usual basic quantal concept of state and equations of motion are also an automatic consequence.

We note that we might also take as basic variational postulate II:

$$\delta \left|\sum_{p \in C} \exp(iS_p/\hbar)\right|^2 \equiv 0, \tag{1'}$$

which, as a literal tautology, though physically more suggestive and leading to the same results, appears rather a weaker condition.

It appears that the above arguments and parallelism can be extended to the case of fields and, under suitably generalized variation processes, yield the Feynman-Schwinger[6] action principle. However, there are still unsettled mathematical problems in this domain, particularly with regard to permissible classes of field functionals, and our investigations are not yet completed. However, whether in the nonrelativistic or relativistic domain, conventional

[4] To the writer, the Lagrangian formulation, however historically secondary, appears conceptually primary as regards clarity and directness of exposition of the basic physical origins of quantum dynamics and derivation of the Schrödinger equations and their interpretation. Insofar as the basic commutators of the Hamiltonian operator formalism appear to be also implied uniquely, it may also be said to be nearest to a theoretical derivation of these since their usual introduction still contains an uncomfortable element of fiat.

[5] I. M. Gel'fand and A. M. Yaglom, J. Math. Phys. **1**, 48 (1960); S. G. Brush, Revs. Modern Phys. **33**, 79 (1961). The first article contains one of the better accessible discussions of problems of strong proofs, rigorous evaluation, and general properties of relevant function space integrals; the second gives a more general view of various uses and approximation techniques, and probably the most extensive collected bibliography now available on related papers and topics.

[6] F. J. Dyson, *Advanced Quantum Mechanics*, Cornell Lectures, 1953.

correspondence principle arguments hinge on considering $\hbar \to 0$ and arguing, heuristically, that only those paths or field histories (the conceptual relativistic analog of paths in field theory) for which $\delta S = 0$ survive destructive interference. Such arguments, again, can neither make explicit the different definitions of states in classical vs quantal theories, nor provide a rigorous and unambiguous transition from one to the other. In point of fact $\hbar$, though it is effectively negligible in various circumstances and of course disappears from classical equations, is never zero in our world; the deciding point appears, rather, to be the issue of whether we assume determinate vs indeterminate paths or histories. Finally, we remark that in the simplest conservative physical system, exp $(iS/\hbar)$ reduces to a primitive de Broglie phase wave so that, in terms of the present synthesis, the developmental history of the principles of quantum theory appears to turn full circle back to its earliest origins.

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Complex Scalar Field in General Relativity

A. DAS
Department of Physics, Jadavpur University, Calcutta, India
(Received 29 June 1962)

This paper introduces complex scalar fields in general relativity to describe charged, gravitating particles with zero spin. A class of exact solutions of the combined Maxwell-Einstein-Klein-Gordon field equations is found that may represent complete models of matter. One of the models discussed is spherically symmetric and the remaining class does not assume any specific symmetry. Such exact solutions are possible only if the mass parameter equals the charge parameter in magnitude, so that physically speaking, matter is in equilibrium under the mutual action of electromagnetic and gravitational forces.

I. INTRODUCTION

In recent years interest has been focussed on a real scalar field without a mass parameter in general relativity.[1] But the scalar (or pseudoscalar) fields that find application in physics are usually complex and always with a mass parameter. In the present paper we shall introduce the complex scalar field satisfying Klein-Gordon equations to replace the phenomenological description of matter in the right-hand sides of electromagnetic and gravitational equations. We have formulated the Cauchy problem of the partial differential equations concerned, and proved the differential conservations of energy-momentum and charge-current in the curved space-time. Description of matter in general relativity by the Dirac field has already been discussed in a less comprehensive way.[2]

In Sec. III we investigate the stationary s-state model of the charged scalar particle which generates electric and metric fields with spherical symmetry. It is shown that under suitable conditions for material equilibrium, the whole set of 16 Maxwell-Einstein-Klein-Gordon equations can be reduced to one Emden type of nonlinear equation. In the nonstatic case it is found that Birkhoff's theorem exists.

In the last section we discuss the models of matter in stationary state with uniform distribution, generating statical electric and metric fields without any particular spatial symmetry. It is shown that under suitable conditions of balance, the Weyl-Majumdar condition[3] $g_{44} = [a \pm (4\pi)^{1/2}A_4]^{-2}$ between the electrostatic potential A_4 and the component of metric tensor g_{44}, follows from the Klein-Gordon equations alone. Also, the whole set of 16 field equations is reduced to one of the form $\nabla^2\varphi = -\lambda\varphi^3$.

Such drastic reduction of number of equations in all cases discussed is only possible if the mass parameter m equals the magnitude of charge parameter ϵ, so that electromagnetic and gravitational forces on matter balance each other. However, the relation is not realized in any known elementary particles and the models presented here are not immediately applicable to physics. Nevertheless the main object, that is to replace the phenomenological description of matter and to construct completely field theoretic singularity-free models, should not be less interesting.

II. THE COMBINED MAXWELL-EINSTEIN-KLEIN-GORDON FIELD EQUATIONS

As for notation, Latin indices stand for space-time components, Greek indices for space only. The summation convention is followed. The signature of the metric form is -2. The covariant and partial differentiations of a tensor component $T::$ are denoted by $\nabla_k T::$ and $\partial_k T::$, respectively. An event and a space point will be denoted by x and $\mathbf{x}$, respectively, and time by $t \equiv x^4$. Units are so chosen that $\hbar = c = G = 1$ and all physical quantities are expressed as pure numbers.

The combined Maxwell-Einstein-Klein-Gordon equations are taken to be[4]

$$B \equiv (D^i D_i + m^2)\psi = 0,$$

$$B^* \equiv (D^{*i} D_i^* + m^2)\psi^* = 0,$$

$$E^i \equiv \nabla_j F^{ij} + (4\pi)^{1/2} i\epsilon(D^{*i}\psi^* \cdot \psi - \psi^* D^i\psi) = 0,$$

$$Q_{ij} \equiv R_{ij} - \tfrac{1}{2}g_{ij}R + 8\pi[D^*_{(i}\psi^* \cdot D_{j)}\psi - g_{ij}(D^{*a}\psi^* \cdot D_a\psi - m^2\psi^*\psi) + E_{ij}] = 0, \quad (2.1)$$

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where,

$$D_i \equiv \nabla_i + (4\pi)^{1/2} i\epsilon A_i, \quad D_i^* \equiv \nabla_i - (4\pi)^{1/2} i\epsilon A_i, \quad \epsilon = \left(\frac{1}{137}\right)^{1/2},$$

$$F_{ij} \equiv \nabla_{[j} A_{i]} \equiv \nabla_j A_i - \nabla_i A_j,$$

$$D^*_{(i}\psi^* \cdot D_{j)}\psi \equiv D^*_i\psi^* \cdot D_j\psi + D^*_j\psi^* \cdot D_i\psi,$$

$$E_{ij} \equiv -F_{ik}F_j^{\ k} + \tfrac{1}{4} g_{ij} F_{ab}F^{ab}.$$

In (2.1), ψ is the complex scalar field which represents matter; A^i is the electromagnetic 4-potential, and R_{ij} is the Ricci tensor. The set of equations (2.1), besides possessing general covariance, is invariant under the gauge transformation

$$\psi' = \psi \exp\left[i(4\pi)^{1/2}\epsilon\Lambda(x)\right],$$
$$\psi^{*\prime} = \psi^* \exp\left[-i(4\pi)^{1/2}\epsilon\Lambda\right],$$
$$A'_a = A_a - \nabla_a \Lambda.$$

The field equations (2.1) are the Euler-Lagrange equations which are obtainable when the action integral

$$A = \int \left[R + 16\pi(D^{*a}\psi^* \cdot D_a\psi - m^2\psi^*\psi) - 4\pi F_{ab}F^{ab}\right](-g)^{1/2}\, d^4x$$

is varied with respect to the 16 variables ψ, ψ^*, A_i, g^{ij}.

The set of equations (2.1) is a determinate system of partial differential equations containing the same number of independent equations as unknowns. In Appendix I we discuss the Cauchy problem for the set of equations (2.1).

In Appendix II we show the differential conservations of symmetrized energy-momentum tensor and charge-current vector of the complex scalar field in the curved space-time.

We shall now rewrite (2.1) in a more suitable form for subsequent use:

$$\begin{aligned}
B &\equiv (-g)^{-1/2}\,\partial_j[(-g)^{1/2}g^{ij}\,\partial_i\psi] \\
&\quad + 2(4\pi)^{1/2} i\epsilon g^{ij} A_i\,\partial_j\psi \\
&\quad + (4\pi)^{1/2} i\epsilon(-g)^{-1/2}\,\partial_j[(-g)^{1/2}g^{ij}A_i]\psi \\
&\quad - 4\pi\epsilon^2 g^{ij}A_iA_j\psi + m^2\psi = 0, \\
B^* &= 0, \\
E^i &\equiv (-g)^{-1/2}\,\partial_j[(-g)^{1/2}g^{ik}g^{jl}(\partial_l A_k - \partial_k A_l)] \\
&\quad + (4\pi)^{1/2} i\epsilon g^{ij}[\partial_j\psi^* \cdot \psi - \psi^*\,\partial_j\psi \\
&\quad - 2(4\pi)^{1/2} i\epsilon A_j\psi^*\psi] = 0, \qquad (2.1')
\end{aligned}$$

$$\begin{aligned}
\tilde{Q}_{ij} &\equiv Q_{ij} - \tfrac{1}{2} g_{ij} Q^k_{\ .k} \\
&\equiv R_{ij} + 8\pi\{[\partial_i\psi^* - (4\pi)^{1/2} i\epsilon A_i\psi^*] \\
&\quad \times [\partial_j\psi + (4\pi)^{1/2} i\epsilon A_j\psi] \\
&\quad + [\partial_j\psi^* - (4\pi)^{1/2} i\epsilon A_j\psi^*] \\
&\quad \times [\partial_i\psi + (4\pi)^{1/2} i\epsilon A_i\psi] - m^2 g_{ij}\psi^*\psi \\
&\quad - g^{kl}(\partial_l A_i - \partial_i A_l)(\partial_k A_j - \partial_j A_k) \\
&\quad + \tfrac{1}{4} g_{ij} g^{ac} g^{bd}(\partial_d A_c - \partial_c A_d)(\partial_b A_a - \partial_a A_b)\} = 0.
\end{aligned}$$

III. A CLASS OF SPHERICALLY SYMMETRIC SOLUTIONS

For the stationary s state of the matter field and statical electric and metric fields with spherical symmetry, we take

$$\psi = R(r)e^{-iEt}, \qquad \psi^* = R(r)e^{iEt}, \qquad A_\alpha = 0, \qquad \varphi \equiv A_4(r) \not\equiv 0,$$

$$(g_{ij}) = \begin{bmatrix} -e^{\lambda(r)} & & & \\ & -r^2 e^{\lambda} & & \\ & & -r^2\sin^2\theta e^{\lambda} & \\ & & & e^{\nu(r)} \end{bmatrix}. \qquad (3.1)$$

Substituting (3.1) into (2.1′), we obtain after straightforward calculation,

$$\begin{aligned}
B &\equiv -e^{-\lambda}\{R'' + (2/r)R' + \tfrac{1}{2}(\lambda' + \nu')R' \\
&\quad + e^{\lambda-\nu}[E - (4\pi)^{1/2}\epsilon\varphi]^2 R - m^2 e^{\lambda} R\}e^{-iEt} = 0, \\
E^\alpha &\equiv 0, \\
E^4 &\equiv -e^{-(\lambda+\nu)}\{\varphi'' + (2/r)\varphi' + \tfrac{1}{2}(\lambda' - \nu')\varphi' \\
&\quad + 2(4\pi)^{1/2}\epsilon\, e^{\lambda}[E - (4\pi)^{1/2}\epsilon\,\varphi]R^2\} = 0, \\
\tilde{Q}_{11} &\equiv \lambda'' + \lambda'/r + \tfrac{1}{2}\nu'' + \tfrac{1}{4}\nu'^2 - \tfrac{1}{4}\lambda'\nu' \\
&\quad + (2R'^2 + m^2 e^{\lambda} R^2 - \tfrac{1}{2}\tilde{e}^{\nu}\varphi'^2) = 0, \qquad (3.2) \\
\tilde{Q}_{22} &\equiv r^2[\tfrac{1}{2}\lambda'' + \tfrac{1}{4}\lambda'^2 + \tfrac{3}{2}\lambda'/r + \tfrac{1}{2}\nu'/r \\
&\quad + \tfrac{1}{4}\lambda'\nu' + 8\pi(m^2 e^{\lambda} R^2 + \tfrac{1}{2}\tilde{e}^{\nu}\varphi'^2)] = 0, \\
\tilde{Q}_{33} &= \tilde{Q}_{22}\sin^2\theta, \\
\tilde{Q}_{44} &\equiv -e^{\nu-\lambda}(\tfrac{1}{2}\nu'' + \tfrac{1}{4}\nu'^2 + \nu'/r + \tfrac{1}{4}\lambda'\nu') \\
&\quad + 8\pi\{2[E - (4\pi)^{1/2}\epsilon\,\varphi]^2 R^2 \\
&\quad - m^2 e^{\nu} R^2 + \tfrac{1}{2}\tilde{e}^{\lambda}\varphi'^2\} = 0, \\
\tilde{Q}_{\alpha 4} &\equiv 0,
\end{aligned}$$

where the prime denotes differentiation with respect to r.

If we write

$$v = e^{\nu/2}, \quad v' = \tfrac{1}{2}e^{\nu/2}\nu', \quad v'' = e^{\nu/2}(\tfrac{1}{2}\nu'' + \tfrac{1}{4}\nu'^2),$$

then $\tilde{Q}_{44} = 0$ becomes

$$v'' + (2/r)v' + \tfrac{1}{2}\lambda' v' = 8\pi\{2v^{-1}[E - (4\pi)^{1/2}\epsilon\,\varphi]^2 e^{\lambda} R^2 - m^2 v e^{\lambda} R^2\} + 4\pi v^{-1}\varphi'^2. \quad (3.3)$$

Without loss of generality we can put

$$v(r) = V[\varphi(r)], \quad v' = V_{\varphi}\varphi', \quad v'' = V_{\varphi}\varphi'' + V_{\varphi\varphi}\varphi'^2,$$
$$V_{\varphi} = dV(\varphi)/d\varphi, \qquad V_{\varphi\varphi} - d^2V/d\varphi^2,$$

and (3.3) becomes

$$\varphi'' + (2/r)\varphi' + \tfrac{1}{2}\lambda'\varphi' = V_{\varphi}^{-1}(4\pi V^{-1} - V_{\varphi\varphi})\varphi'^2 + 8\pi V_{\varphi}^{-1} e^{\lambda} R^2\{2V^{-1}[E - (4\pi)^{1/2}\epsilon\,\varphi]^2 - m^2 V\}. \quad (3.4)$$

Similarly $E^4 = 0$ becomes

$$\varphi'' + (2/r)\varphi' + \tfrac{1}{2}\lambda'\varphi' = V^{-1}V_{\varphi}\varphi'^2 - 2(4\pi)^{1/2}\epsilon\, e^{\lambda} R^2[E - (4\pi)^{1/2}\epsilon\,\varphi]. \quad (3.5)$$

Subtracting (3.4) from (3.5), we obtain

$$[4\pi(VV_{\varphi})^{-1} - V_{\varphi\varphi}V_{\varphi}^{-1} - V^{-1}V_{\varphi}]\varphi'^2 + [8\pi V_{\varphi}^{-1}\{2[E - (4\pi)^{1/2}\epsilon\,\varphi]^2 V^{-1} - m^2 V\} + 2(4\pi)^{1/2}\epsilon\{E - (4\pi)^{1/2}\epsilon\,\varphi\}]e^{\lambda} R^2 = 0. \quad (3.6)$$

We shall now specify a class of solutions which satisfy (3.6) by virtue of

$$4\pi(VV_{\varphi})^{-1} - V_{\varphi\varphi}V_{\varphi}^{-1} - V^{-1}V_{\varphi} = 0, \quad (3.7a)$$

$$8\pi V_{\varphi}^{-1}\{2V^{-1}[E - (4\pi)^{1/2}\epsilon\,\varphi]^2 - m^2 V\} + 2(4\pi)^{1/2}\epsilon[E - (4\pi)^{1/2}\epsilon\,\varphi] = 0. \quad (3.7b)$$

Integration of (3.7a) yields Weyl's condition[5]

$$e^{\nu(r)} = V(\varphi) = a + 2b\varphi(r) + 4\pi[\varphi(r)]^2, \quad (3.8)$$

a, b being constants of integration.

Substituting (3.8) into (3.7b) and equating the coefficients of $[\varphi(r)]^n$, $(n = 2, 1, 0)$ to zero we get

$$\epsilon^2 = m^2, \qquad b = -(4\pi)^{1/2}E/\epsilon, \qquad a = (E/m)^2. \quad (3.9)$$

Thus we get from (3.8) and (3.9) the Weyl-Majumdar condition

$$m^2 e^{\nu} = [E - (4\pi)^{1/2}\epsilon\,\varphi]^2. \quad (3.10)$$

Substituting (3.10) into (3.2) and remembering

$$\tfrac{1}{2}e^{-\nu}\varphi'^2 = (1/32\pi)\nu'^2,$$

we obtain

$$-e^{\lambda+iE^1}B \equiv R'' + (2/r)R' + \tfrac{1}{2}(\lambda' + \nu')R' = 0,$$
$$\tilde{Q}_{11} \equiv \lambda'' + \lambda'/r + \tfrac{1}{2}\nu'' - \tfrac{1}{4}\lambda'\nu' + 8\pi(2R'^2 + m^2 e^{\lambda} R^2) = 0,$$
$$r^{-2}\tilde{Q}_{22} \equiv \tfrac{1}{2}\lambda'' + \tfrac{1}{4}\lambda'^2 + \tfrac{3}{2}\lambda'/r + \tfrac{1}{2}\nu'/r + \tfrac{1}{4}\lambda'\nu' + \tfrac{1}{4}\nu'^2 + 8\pi m^2 e^{\lambda} R^2 = 0, \quad (3.11)$$
$$-e^{\lambda-\nu}\tilde{Q}_{44} \equiv \tfrac{1}{2}\nu'' + \nu'/r + \tfrac{1}{4}\lambda'\nu' - 8\pi m^2 e^{\lambda} R^2 = 0.$$

Rearranging the equations slightly, we get

$$\tilde{Q}_{11} - e^{\lambda-\nu}\tilde{Q}_{44} \equiv (\lambda'' + \nu'') + (1/r)(\lambda' + \nu') + 16\pi R'^2 = 0, \quad (3.12a)$$

$$2r^{-2}\tilde{Q}_{22} - 2e^{\lambda-\nu}\tilde{Q}_{44} \equiv (\lambda'' + \nu'') + (3/r)(\lambda' + \nu') + \tfrac{1}{2}(\lambda' + \nu')^2 = 0. \quad (3.12b)$$

The solution of (3.12b) is

$$\lambda + \nu = 2\ln(1 - r_0^2/r^2), \quad (3.13)$$

where we have demanded $\lambda + \nu \to 0$ as $r \to \infty$ and r_0 is the constant of integration.

With (3.13), integration of (3.12a) yields

$$R = \left(\frac{1}{8\pi}\right)^{1/2} \ln\left(\frac{r - r_0}{r + r_0}\right), \quad (3.14)$$

where we have demanded $R \to 0$ as $r \to \infty$.

The solution (3.14) satisfies $B = 0$ automatically and $\tilde{Q}_{44} = 0$ goes over into

$$\nu'' + \frac{2}{r}\nu' - \tfrac{1}{2}\nu'^2 + \frac{2r_0^2\nu'}{r(r^2 - r_0^2)} = 2m^2 e^{-\nu}\left[\left(1 - \frac{r_0^2}{r^2}\right)\ln\left(\frac{r - r_0}{r + r_0}\right)\right]^2. \quad (3.15)$$

Substituting $\rho = \ln[(r - r_0)/(r + r_0)]$ and $\nu(r) = -2\ln\chi(\rho)$, we obtain from (3.15)

$$d^2\chi/d\rho^2 = -4m^2 r_0^2(\rho\ \mathrm{csch}^2\,\rho)^2\chi^3. \quad (3.16)$$

If we take r_0 in (3.13) to be zero, from $B = 0$, R becomes a constant which can be normalized to unity. Finally, with $R = 1$, $\tilde{Q}_{44} = 0$ becomes

$$\nu'' + (2/r)\nu' - \tfrac{1}{2}\nu'^2 = 16\pi m^2 e^{-\nu}. \quad (3.17)$$

Substituting $\nu = -2\ln\xi$, we obtain an Emden equation

$$\xi'' + (2/r)\xi' = -8\pi m^2\xi^3. \quad (3.18)$$

This is a special case of the class of solutions to be discussed in the following section. It may be mentioned that the metrical universe implied by the Emden equation (3.18) is finite and closed.[6]

[5] See reference 3.

[6] See reference 2.

For the case of nonstatic spherical symmetry, we take

$$\psi = \psi(r, t),\ F_{24} = F_{34} = F_{\alpha\beta} = 0,\ F_{14} \neq 0,$$
$$ds^2 = -e^{\lambda(r,t)}\,dr^2 - r^2\,d\theta^2 - r^2\sin^2\theta\,d\varphi^2 + e^{\nu(r,t)}\,dt^2. \tag{3.19}$$

We have excluded the unphysical radial magnetic field so that

$$F_{\alpha\beta} \equiv \partial_\beta A_\alpha - \partial_\alpha A_\beta = 0, \qquad A_\alpha = \partial_\alpha \Lambda. \tag{3.20}$$

Now making a gauge transformation

$$A'_\alpha = A_\alpha - \partial_\alpha\Lambda, \qquad \psi' = \psi \exp[i(4\pi)^{1/2}\epsilon\Lambda],$$
$$\psi^{*\prime} = \psi^* \exp[-i(4\pi)^{1/2}\epsilon\Lambda],$$

and dropping the prime, subsequently we have from (3.19) and (3.20)

$$\psi = \psi(r, t),\quad A_\alpha = 0,\quad \varphi \equiv A_4(r, t) \neq 0, \tag{3.21}$$
$$ds^2 = -e^{\lambda(r,t)}\,dr^2 - r^2\,d\theta^2 - r^2\sin^2\theta\,d\varphi^2 + e^{\nu(r,t)}\,dt^2. \tag{2.1}$$

If we restrict the matter field to the stationary s state, then

$$\psi = R(r)e^{-iEt}, \qquad \psi^* = R(r)e^{iEt}. \tag{3.22}$$

With (3.21) and (3.22), $E^2 = E^3 = \tilde{Q}_{24} = \tilde{Q}_{34} = 0$ are identically satisfied and $\tilde{Q}_{14} = 0$ gives

$$\partial_4\lambda = 0. \tag{3.23}$$

To satisfy $E^1 = 0$ identically, we assume the Lorentz gauge condition

$$\nabla_i A^i = 0, \tag{3.24}$$

so that

$$E^i \equiv \nabla^i\nabla_j A^i - R^{ij}A_j + (4\pi)^{1/2}i\epsilon(D^{*i}\psi^*\cdot\psi - \psi^* D^i\psi) = 0. \tag{3.25}$$

From (3.21), (3.22), (3.23), and (3.25) it is easy to see that $E^1 = 0$ is automatically satisfied.

Now there will remain five equations $B = E^4 = \tilde{Q}_{11} = \tilde{Q}_{22} = \tilde{Q}_{44} = 0$ for four unknowns R, φ, λ, ν. We note that $B = 0$ is a consequence of the other four field equations $E^4 = \tilde{Q}_{11} = \tilde{Q}_{22} = \tilde{Q}_{44} = 0$, and these, by virtue of (3.21), (3.22), and (3.23), contain no explicit time derivative at all. Thus we conclude that in the present case, Birkhoff's theorem exists, that is, spherically symmetric metric and electromagnetic fields generated by the stationary matter field in the s state are essentially static.

IV. A CLASS OF EXACT SOLUTIONS WITHOUT ANY SPECIFIC SYMMETRY

For matter at rest generating the most general type of statical metric and electrostatic fields, we can take

$$\psi = e^{-imt},\quad \psi^* = e^{imt},\quad A_\alpha = 0,\quad \varphi \equiv A_4(\mathbf{x}) \neq 0,\quad F_{4\alpha} = \partial_\alpha\varphi, \tag{4.1}$$
$$ds^2 = g_{\alpha\beta}(\mathbf{x})\,dx^\alpha\,dx^\beta + f(\mathbf{x})\,dt^2.$$

From (2.1′) and (4.1), remembering $g^{44} = f^{-1}$, $\Gamma^4_{\alpha\beta} = \Gamma^\alpha_{4\beta} = \Gamma^4_{44} = 0$, $B = 0$ leads to

$$B \equiv -m^2 f^{-1} + 2(4\pi)^{1/2}\epsilon\, mf^{-1}\varphi - 4\pi\epsilon^2 f^{-1}\varphi + m^2 = 0,$$
$$f = [1 - (4\pi)^{1/2}(\epsilon/m)\varphi]^2, \tag{4.2}$$
$$f_\varphi \equiv df/d\varphi = -2(4\pi)^{1/2}(\epsilon/m)f^{1/2},$$
$$f_{\varphi\varphi} = 8\pi\epsilon^2/m^2.$$

Thus, we have obtained Weyl-Majumdar type of condition[7] from the Klein-Gordon equation alone without having recourse to the electro-gravitational equations.

Now, from (2.1′) and (4.1) $E^\alpha = 0$ identically and $E^4 = 0$ gives

$$E^4 \equiv (-g)^{-1/2}\,\partial_\alpha[f^{-1}(-g)^{1/2}g^{\alpha\beta}\,\partial_\beta\varphi] - 2(4\pi)^{1/2}\epsilon mf^{-1}[1 - (4\pi)^{1/2}(\epsilon/m)\varphi] = 0. \tag{4.3}$$

Remembering (4.2) the last equation goes over into

$$(-g)^{-1/2}\,\partial_\alpha[(-g)^{1/2}g^{\alpha\beta}\,\partial_\beta\varphi] = f^{-1}f_\varphi g^{\alpha\beta}\,\partial_\alpha\varphi\cdot\partial_\beta\varphi + 2(4\pi)^{1/2}\epsilon mf^{1/2}. \tag{4.4}$$

With (4.1), (4.2) we have for the Christoffel symbols

$$\Gamma^4_{\alpha\beta} = \Gamma^\alpha_{\beta 4} = \Gamma^4_{44} = 0, \qquad \Gamma^\alpha_{44} = \tfrac{1}{2}g^{\alpha\beta}f_\varphi\,\partial_\beta\varphi, \qquad \Gamma^4_{\alpha 4} = \tfrac{1}{2}f^{-1}f_\varphi\,\partial_\alpha\varphi,$$

so that

$$R_{44} = -\Gamma^\alpha_{44}\,\partial_\alpha \ln(-g)^{1/2} - \partial_\alpha\Gamma^\alpha_{44} + 2\Gamma^\alpha_{44}\Gamma^4_{\alpha 4}$$
$$= \tfrac{1}{2}f_\varphi(-g)^{-1/2}\,\partial_\alpha[(-g)^{1/2}g^{\alpha\beta}\,\partial_\beta\varphi] + \tfrac{1}{2}(f_{\varphi\varphi} - f^{-1}f_\varphi^2)g^{\alpha\beta}\,\partial_\alpha\varphi\cdot\partial_\beta\varphi. \tag{4.5}$$

From (2.1′), (4.1), (4.2), and (4.5), we have $\tilde{Q}_{\alpha 4} = 0$ identically, and $\tilde{Q}_{44} = 0$ yields

$$(-g)^{-1/2}\,\partial_\alpha[(-g)^{1/2}g^{\alpha\beta}\,\partial_\beta\varphi] = (f_\varphi)^{-1}(8\pi + f^{-1}f_\varphi^2 - f_{\varphi\varphi})g^{\alpha\beta}\,\partial_\alpha\varphi\cdot\partial_\beta\varphi - 16\pi m^2 f(f_\varphi)^{-1}. \tag{4.6}$$

[7] See reference 3.

In view of (4.2), subtraction of (4.4) from (4.6) leads to

$$(\epsilon^2/m^2 - 1)\{2m^2[1 - (4\pi)^{1/2}(\epsilon/m)\varphi] - g^{\alpha\beta}\,\partial_\alpha\varphi\cdot\partial_\beta\varphi[1 - (4\pi)^{1/2}(\epsilon/m)\varphi]^{-1}\} = 0. \quad (4.7)$$

In general, the last factor in (4.7) would not vanish everywhere, so that we have

$$\epsilon^2 = m^2, \qquad f = [1 \mp (4\pi)^{1/2}\varphi]^2. \quad (4.8)$$

Now, we shall write without loss of generality

$$ds^2 = -\bar{e}^\omega(\bar{g}_{\alpha\beta}\,dx^\alpha\,dx^\beta) + e^\omega\,dt^2. \quad (4.9)$$

From (2.1′), (4.1), (4.8), and (4.9), equations $\tilde{Q}_{\alpha\beta} = 0$, $\tilde{Q}_{44} = 0$ yield, respectively (see Appendix III),

$$\tilde{Q}_{\alpha\beta} \equiv \bar{R}_{\alpha\beta} - \tfrac{1}{2}\bar{g}_{\alpha\beta}(\bar{\nabla}^\gamma\bar{\nabla}_\gamma\omega - \tfrac{1}{2}\bar{\nabla}^\gamma\omega\cdot\bar{\nabla}_\gamma\omega - 16\pi m^2\bar{e}^\omega) = 0, \quad (4.10a)$$

$$\tilde{Q}_{44} \equiv -\tfrac{1}{2}e^{2\omega}(\bar{\nabla}^\gamma\bar{\nabla}_\gamma\omega - \tfrac{1}{2}\bar{\nabla}^\gamma\omega\cdot\bar{\nabla}_\gamma\omega - 16\pi m^2\bar{e}^\omega) = 0, \quad (4.10b)$$

where the bar refers to the 3-space V_3 with metric $\bar{g}_{\alpha\beta}$.

Comparing (4.10a) and (4.10b) we have

$$\bar{R}_{\alpha\beta} = 0 \quad (4.11)$$

or, in other words the V_3 is flat, because in a 3-space the curvature tensor can be expressed algebraically in terms of a Ricci tensor each having six components. So we can choose $\bar{g}_{\alpha\beta} = \delta_{\alpha\beta}$ and (4.10b) reduces to

$$\partial_\gamma\,\partial_\gamma\omega - \tfrac{1}{2}\,\partial_\gamma\omega\cdot\partial_\gamma\omega = 16\pi m^2\bar{e}^\omega. \quad (4.12)$$

Substituting $\omega = -2\ln(1 + \Omega)$, we get from (4.12)

$$\nabla^2\Omega \equiv \partial_\gamma\,\partial_\gamma\Omega = -8\pi m^2(1 + \Omega)^3. \quad (4.13)$$

In the one-dimensional problem the solution of (4.13) in terms of elliptic functions is

$$1 + \Omega(x^1) = -A\,\mathrm{dn}\,\{2A[(2\pi)^{1/2}mx^1 + B], \tfrac{1}{2}\} \quad (4.14)$$

A, B being constants of integration. In the case of spherical symmetry, the solution of (4.13) is an Emden function as mentioned in the previous section.

Finally, we summarize this class of exact solutions of (2.1) by the following:

$$ds^2 = -(1 + \Omega)^2[(dx^1)^2 + (dx^2)^2 + (dx^3)^2] + (1 + \Omega)^{-2}\,dt^2,$$
$$\psi = e^{-imt}, \quad \psi^* = e^{imt}, \quad A_\alpha = 0,$$
$$A_4 = \pm\frac{1}{(4\pi)^{1/2}}\frac{\Omega}{1 + \Omega}, \quad (4.15)$$
$$\epsilon^2 = m^2, \quad \nabla^2\Omega = -8\pi m^2(1 + \Omega)^3.$$

By applying a Lorentz transformation to this system, the matter field can be brought into the plane wave form and the metric and electromagnetic fields into nonstatic forms.

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APPENDIX I

We shall formulate here the Cauchy problem for the set of partial differential equations (2.1).

Equations (2.1) contain 16 unknowns exhibited as follows:

$$1(\mathrm{Re}\,\psi) + 1(\mathrm{Im}\,\psi) + 4(A^i) + 10(g_{ij}).$$

Since one subsidiary condition $S = 0$ on the 4-potential A_i and four coordinate conditions $C_i = 0$ can be imposed, there are 21 equations in total, namely,

$$1(B) + 1(B^*) + 4(E^i) + 10(Q_{ij}) + 1(S) + 4(C_i).$$

However, there are five identities

$$4(\nabla_i Q^{ij} = 0) + 1(\nabla_i E^i = 0).$$

Therefore, the number of independent equations is 16 and the system of partial differential equations under consideration is determinate.

Now we shall need two lemmas which we shall state without proof.[8]

Lemma I. If $W_{ij} = W_{ji}$, $\nabla_i W^{ij} = 0$, $\bar{W}_{ij} \equiv W_{ij} - \tfrac{1}{2}g_{ij}W^k_{\cdot k}$, the statements

(i) $W_{ij} = 0$ in space-time S_4,
(ii) $\bar{W}_{\alpha\beta} = 0$ in S_4, $W^4_{\cdot k} = 0$ in the initial hypersurface S_3 with $t = 0$,

are equivalent.

Lemma II. If $\nabla_i U^i = 0$, the statements

(i) $U^i = 0$ in S_4,
(ii) $U^\alpha = 0$ in S_4, $U^4 = 0$ in S_3,

are equivalent.

Because of these two lemmas, the field equations (2.1) are equivalent to

$$R_{\alpha\beta} + 8\pi(D^*_{(\alpha}\psi^*\cdot D_{\beta)}\psi - m^2 g_{\alpha\beta} + E_{\alpha\beta}) = 0,$$
$$\nabla_i\nabla^{[i}A^{\alpha]} + (4\pi)^{1/2}ie(D^{*\alpha}\psi^*\cdot\psi - \psi^*\,D^\alpha\psi) = 0, \quad (I.1)$$
$$(D^i\,D_i + m^2)\psi = 0,$$
$$(D^{*i}\,D^*_i + m^2)\psi^* = 0$$

[8] J. L. Synge, *Relativity: The General Theory* (North-Holland Publishing Company, Amsterdam, 1960), p. 211.

in S_4 and

$$R^4_{\cdot\alpha} + 8\pi(D^{*4}\psi^*\cdot D_\alpha\psi + D^*_\alpha\psi^*\cdot D^4\psi + E^4_{\cdot\alpha}) = 0,$$
$$R^4_{\cdot 4} - \tfrac{1}{2}R + 8\pi(D^{*4}\psi^*\cdot D_4\psi - D^{*\alpha}\psi^*\cdot D_\alpha\psi + m^2\psi^*\psi + E^4_{\cdot 4}) = 0, \quad \text{(I.2)}$$
$$\nabla_i\nabla^{[i}A^{4]} + (4\pi)^{1/2}i\epsilon(D^{*4}\psi^*\cdot\psi - \psi^* D^4\psi) = 0$$

in S_3.

We choose the normal Gaussian coordinates to exploit the coordinate conditions and a subsidiary condition so that

$$g^{\alpha 4} = g_{\alpha 4} = 0,\ g^{44} = g_{44} = 1,\ A^4 = A_4 = 0. \quad \text{(I.3)}$$

Now in the normal Gaussian coordinates we have

$$R_{\alpha\beta} = \bar{R}_{\alpha\beta} + \tfrac{1}{2}\,\partial_4^2 g_{\alpha\beta} + \tfrac{1}{4}A\,\partial_4 g_{\alpha\beta} - \tfrac{1}{2}g^{\mu\nu}\,\partial_4 g_{\mu\alpha}\cdot\partial_4 g_{\nu\beta},$$
$$G_{\mu 4} = R_{\mu 4} = \tfrac{1}{2}\,\partial_\mu A - \tfrac{1}{2}\bar{\nabla}^\sigma(\partial_4 g_{\mu\sigma}), \quad \text{(I.4)}$$
$$G_{44} = -\tfrac{1}{2}\bar{R} - \tfrac{1}{8}A^2 + \tfrac{1}{8}B.$$

The explanation of the symbols is as follows:

$\bar{R}_{\mu\nu}$ = Ricci subtensor of a hypersurface t = const,
$\bar{R}$ = curvature subinvariant of t = const,
$\bar{G}_{\mu\nu}$ = Einstein subtensor of t = const,
$\bar{\nabla}_\mu$ = operator of covariant differentiation in t = const,

$$A = g^{\mu\nu}\,\partial_4 g_{\mu\nu}, \qquad B = g^{\mu\nu}g^{\rho\sigma}\,\partial_4 g_{\mu\rho}\cdot\partial_4 g_{\nu\sigma}.$$

From (I.1), (I.3) and (I.4) we get

$$\partial_4^2 g_{\alpha\beta} = -2\bar{R}_{\alpha\beta} - \tfrac{1}{2}A\,\partial_4 g_{\alpha\beta} + g^{\mu\nu}\,\partial_4 g_{\mu\alpha}\cdot\partial_4 g_{\nu\beta} - 16\pi[D^*_{(\alpha}\psi^*\cdot D_{\beta)}\psi - m^2 g_{\alpha\beta}\psi^*\psi - g^{\gamma\delta}\,\partial_{[\gamma}A_{\alpha]}\,\partial_{[\delta}A_{\beta]} + \tfrac{1}{4}g_{\alpha\beta}g^{\mu\gamma}g^{\nu\delta}\,\partial_{[\nu}A_{\mu]}\,\partial_{[\delta}A_{\gamma]}],$$
$$\partial_4^2 A_\alpha = g^{\beta\gamma}\,\partial_4 g_{\alpha\gamma}\cdot\partial_4 A_\beta - \partial_4 \ln(-g)^{1/2}\cdot\partial_4 A_\alpha - g_{\alpha\sigma}\bar{\nabla}_\beta\nabla^{[\beta}A^{\sigma]} - (4\pi)^{1/2}i\epsilon(D^*_\alpha\psi^*\cdot\psi - \psi^* D_\alpha\psi),$$
$$\partial_4^2\psi = -(D^\alpha D_\alpha + m^2)\psi - \partial_4\psi\cdot\partial_4 \ln(-g)^{1/2},$$
$$\partial_4^2\psi^* = -(D^{*\alpha} D^*_\alpha + m^2)\psi^* - \partial_4\psi^*\cdot\partial_4 \ln(-g)^{1/2}. \quad \text{(I.5)}$$

We shall now choose for the Cauchy data on the initial hypersurface S_3, the following 22 quantities:

$$g_{\alpha\beta},\ \xi_{\alpha\beta} \equiv \partial_4 g_{\alpha\beta};\quad A_\alpha,\ \chi_\alpha \equiv \partial_4 A_\alpha;$$
$$\psi,\ \eta \equiv \partial_4\psi;\quad \psi^*,\ \eta^* \equiv \partial_4\psi^*.$$

In terms of the Cauchy data (I.5) become

$$\partial_4^2 g_{\alpha\beta} = \text{C.D.},\quad \partial_4^2 A_\alpha = \text{C.D.},\quad \partial_4^2\psi = \text{C.D.},\quad \partial_4^2\psi^* = \text{C.D.}, \quad \text{(I.6)}$$

in S_3.

The Equations (I.2) become

$$\bar{\nabla}_\alpha\xi^\mu_{\cdot\mu} - \bar{\nabla}^\sigma\xi_{\alpha\sigma} + 16\pi\{\eta^*[\partial_\alpha\psi + (4\pi)^{1/2}i\epsilon A_\alpha\psi] + [\partial_\alpha\psi^* - (4\pi)^{1/2}i\epsilon A_\alpha\psi^*]\eta - g^{\beta\gamma}\chi_\beta\,\partial_{[\gamma}A_{\alpha]}\} = 0,$$
$$\bar{R} + \tfrac{1}{4}(\xi^\mu_{\cdot\mu})^2 - \tfrac{1}{4}\xi^\mu_{\cdot\nu}\xi^\nu_{\cdot\mu} + 16\pi\{\eta^*\eta - g^{\alpha\beta}[\partial_\alpha\psi^* - (4\pi)^{1/2}i\epsilon A_\alpha\psi^*] \times [\partial_\beta\psi + (4\pi)^{1/2}i\epsilon A_\beta\psi] - \tfrac{1}{2}\chi^\alpha\chi_\alpha + \tfrac{1}{2}g^{\alpha\mu}g^{\beta\nu}\,\partial_{[\beta}A_{\alpha]}\,\partial_{[\nu}A_{\mu]}] = 0, \quad \text{(I.7)}$$
$$\bar{\nabla}_\alpha\chi^\alpha - (4\pi)^{1/2}i\epsilon(\eta^*\psi - \psi^*\eta) = 0,$$

in S_3 which are the consistency conditions to be satisfied by the Cauchy data.

Since (I.6) explicitly gives the values of the derivatives of the Cauchy data, in terms of the Cauchy data themselves, we know that a solution exists in the neighborhood of $t = 0$, provided the Cauchy data are chosen to satisfy (I.7).

The solution will read

$$g_{\alpha\beta} = (g_{\alpha\beta})_0 + t(\partial_4 g_{\alpha\beta})_0 + \tfrac{1}{2}t^2(\partial^2 g_{\alpha\beta})_0 + \cdots,$$
$$A_\alpha = (A_\alpha)_0 + t(\partial_4 A_\alpha)_0 + \tfrac{1}{2}t^2(\partial^2 A_\alpha)_0 + \cdots,$$
$$\psi = (\psi)_0 + t(\partial_4\psi)_0 + \tfrac{1}{2}t^2(\partial^2\psi)_0 + \cdots,$$
$$\psi^* = (\psi^*)_0 + t(\partial_4\psi^*)_0 + \tfrac{1}{2}t^2(\partial^2\psi^*)_0 + \cdots.$$

The set of consistency conditions (I.7) is a highly redundant system; only five equations for 12 unknowns. It looks as if it would be easy to satisfy them but in fact this is not so.

APPENDIX II

In this section we shall show the exact differential conservations of charge-current and energy-momentum in the curved space-time. The charge-current vector in (2.1) is

$$S^i \equiv -(4\pi)^{1/2}i\epsilon(D^{*i}\psi^*\cdot\psi - \psi^* D^i\psi). \quad \text{(II.1)}$$

Therefore,

$$[i/(4\pi)^{1/2}\epsilon]\nabla_i S^i = \nabla_i D^{*i}\psi^*\cdot\psi + D^{*i}\psi^*\cdot\nabla_i\psi - \text{c.c.} = D^*_i D^{*i}\psi^*\cdot\psi + D^{*i}\psi^*\cdot D_i\psi - \text{c.c.} = -m^2\psi^*\psi - \text{c.c.} = 0, \quad \text{(II.2)}$$

where we have utilized $B = B^* = 0$.

The symmetrized energy-momentum tensor in (2.1) is

$$\theta^{ij} \equiv D^{*i}\psi^*\cdot D^j\psi + D^{*j}\psi^*\cdot D^i\psi - g^{ij}\, D^{*k}\psi^*\cdot D_k\psi + m^2 g^{ij}\psi^*\psi - F^{ik}F^j_{\cdot k} + \tfrac{1}{4}g^{ij}F^{ab}F_{ab}. \quad \text{(II.3)}$$

Therefore,

$$\begin{aligned}\nabla_j\theta^{ij} &= (\nabla_j\, D^{*i}\psi^*\cdot D^j\psi \\ &\quad + D^{*i}\psi^*\cdot\nabla_j\, D^j\psi - \nabla^i\, D^{*j}\psi^*\cdot D_j\psi + \text{c.c.}) \\ &\quad + m^2\nabla^i(\psi^*\psi) - F^i_{\cdot k}\nabla_j F^{jk} \\ &= (D_j^*\, D^{*i}\psi^*\cdot D^j\psi + D^{*j}\psi^*\cdot D_j\, D^i\psi \\ &\quad - D^{*i}\, D^{*j}\psi^*\cdot D_j\psi + \text{c.c.}) \\ &\quad + m^2(\nabla^i\psi^*\cdot\psi + \psi^*\nabla^i\psi) \\ &\quad - (4\pi)^{1/2}i\epsilon F^i_{\cdot j}(D^{*j}\psi^*\cdot\psi - \psi^*\, D^j\psi) \\ &= (D^{*[j}\, D^{*i]}\psi^*\cdot D_j\psi \\ &\quad + \text{c.c.}) + m^2(-D^{*i}\psi^*\cdot\psi \\ &\quad - \psi^*\, D^i\psi + \nabla^i\psi^*\psi + \psi^*\nabla^i\psi) \\ &\quad - (4\pi)^{1/2}i\epsilon F^{ij}(D_j^*\psi^*\cdot\psi - \psi^*\, D_j\psi) = 0, \quad \text{(II.4)}\end{aligned}$$

where we have utilized

$$B = B^* = 0, \qquad \nabla_{[i}F_{jk]} = 0,$$
$$D^{[j}\, D^{i]}\psi = (4\pi)^{1/2}i\epsilon F^{ij}\psi.$$

APPENDIX III

We can represent a statical universe by

$$ds^2 = g_{\alpha\beta}(\mathbf{x})\, dx^\alpha\, dx^\beta + e^{\omega(x)}\, dt^2. \quad \text{(III.1)}$$

Without loss of generality we can also write

$$ds^2 = -\bar{e}^\omega(\bar{g}_{\alpha\beta}\, dx^\alpha\, dx^\beta) + e^\omega\, dt^2 \quad \text{(III.2)}$$

From (III.1) and (III.2) we have

$$\begin{aligned}&g_{\alpha\beta} = -\bar{e}^\omega\bar{g}_{\alpha\beta}, \quad g_{\alpha 4} = 0, \quad g_{44} = e^\omega, \\ &g^{\alpha\beta} = -e^\omega\bar{g}^{\alpha\beta}, \; g^{\alpha 4} = 0, \; g^{44} = \bar{e}^\omega, \; (-g)^{1/2} = \bar{e}^\omega(\bar{g})^{1/2}, \\ &[\alpha\beta,\gamma] = -\bar{e}^\omega[\overline{\alpha\beta,\gamma}] + \tfrac{1}{2}\bar{e}^\omega(\bar{g}_{\beta\gamma}\,\partial_\alpha\omega + \bar{g}_{\gamma\alpha}\,\partial_\beta\omega - \bar{g}_{\alpha\beta}\,\partial_\gamma\omega), \quad \text{(III.3)} \\ &[44,\alpha] = -[\alpha 4, 4] = -\tfrac{1}{2}e^\omega\,\partial_\alpha\omega, \\ &\Gamma^\mu_{\alpha\beta} = \bar{\Gamma}^\mu_{\alpha\beta} - \tfrac{1}{2}(\delta^\mu_{\cdot\beta}\,\partial_\alpha\omega + \delta^\mu_{\cdot\alpha}\,\partial_\beta\omega - \bar{g}^{\mu\gamma}\bar{g}_{\alpha\beta}\,\partial_\gamma\omega), \\ &\Gamma^4_{\alpha 4} = \tfrac{1}{2}\,\partial_\alpha\omega, \quad \Gamma^\alpha_{44} = \tfrac{1}{2}g^{\alpha\beta}e^{2\omega}\,\partial_\beta\omega,\end{aligned}$$

where the bar indicates the subtensors and other quantities pertaining to the 3-space with the metric $\bar{g}_{\alpha\beta}$. Throughout these calculations we find that the presence of an odd number of suffix 4 destroys a term.

Now, the Ricci tensor is

$$R_{ij} \equiv \partial_i\,\partial_j \ln(-g)^{1/2} - \partial_k\Gamma^k_{ij} + \Gamma^m_{in}\Gamma^n_{mj} - \Gamma^k_{ij}\,\partial_k \ln(-g)^{1/2}. \quad \text{(III.4)}$$

By virtue of (III.3) and (III.4), it follows, after some calculations, that

$$\begin{aligned}&R_{\alpha\beta} = \bar{R}_{\alpha\beta} + \tfrac{1}{2}\bar{\nabla}_\alpha\omega\cdot\bar{\nabla}_\beta\omega - \tfrac{1}{2}\bar{g}_{\alpha\beta}\bar{\nabla}_\gamma\bar{\nabla}^\gamma\omega, \\ &R_{\alpha 4} = 0, \quad \text{(III.5)} \\ &R_{44} = -\tfrac{1}{2}e^{2\omega}\bar{\nabla}_\gamma\bar{\nabla}^\gamma\omega.\end{aligned}$$

Remembering (4.1) and (4.9), we have from the definition of electromagnetic stress tensor after (2.1)

$$\begin{aligned}&E_{\alpha\beta} = -\bar{e}^\omega\,\partial_\alpha\varphi\cdot\partial_\beta\varphi + \tfrac{1}{2}\bar{e}^\omega\bar{g}_{\alpha\beta}\bar{g}^{\gamma\delta}\,\partial_\gamma\varphi\cdot\partial_\delta\varphi, \\ &E_{\alpha 4} = 0, \quad \text{(III.6)} \\ &E_{44} = \tfrac{1}{2}e^\omega\bar{g}^{\alpha\beta}\,\partial_\alpha\varphi\cdot\partial_\beta\varphi.\end{aligned}$$

From (4.8) and (4.9) we notice

$$\begin{aligned}&e^\omega = [1 \mp (4\pi)^{1/2}\varphi]^2, \\ &\bar{e}^{\omega/2}\,\partial_\alpha\varphi = \mp[1/2(4\pi)^{1/2}]\,\partial_\alpha\omega \\ &\qquad = \mp[1/2(4\pi)^{1/2}]\bar{\nabla}_\alpha\omega. \quad \text{(III.7)}\end{aligned}$$

Therefore, (III.6) becomes

$$\begin{aligned}&E_{\alpha\beta} = -(1/16\pi)(\bar{\nabla}_\alpha\omega\cdot\bar{\nabla}_\beta\omega - \tfrac{1}{2}\bar{g}_{\alpha\beta}\bar{\nabla}^\gamma\omega\cdot\bar{\nabla}_\gamma\omega), \\ &E_{\alpha 4} = 0, \quad \text{(III.8)} \\ &E_{44} = (1/32\pi)e^{2\omega}\bar{\nabla}^\gamma\omega\cdot\bar{\nabla}_\gamma\omega.\end{aligned}$$

Now, from (II.3)

$$\tilde{\theta}_{ij} \equiv \theta_{ij} - \tfrac{1}{2}g_{ij}\theta^k_{\cdot k} \equiv D_i^*\psi^*\cdot D_j\psi + D_j^*\psi^*\cdot D_i\psi - m^2 g_{ij}\psi^*\psi + E_{ij}.$$

Therefore we obtain from (4.1), (III.2), (III.7), and (III.8)

$$\begin{aligned}&-8\pi\tilde{\theta}_{\alpha\beta} = -8\pi m^2\bar{e}^\omega\bar{g}_{\alpha\beta} + \tfrac{1}{2}\bar{\nabla}_\alpha\omega\cdot\bar{\nabla}_\beta\omega - \tfrac{1}{4}\bar{g}_{\alpha\beta}\bar{\nabla}^\gamma\omega\cdot\bar{\nabla}_\gamma\omega, \quad \text{(III.9)} \\ &-8\pi\tilde{\theta}_{\alpha 4} = 0, \\ &-8\pi\tilde{\theta}_{44} = -8\pi m^2 e^\omega - \tfrac{1}{4}e^{2\omega}\bar{\nabla}^\gamma\omega\cdot\bar{\nabla}_\gamma\omega.\end{aligned}$$

Combining (III.5) and (III.9) in the equations $\tilde{Q}_{\alpha\beta} = 0$, $\tilde{Q}_{44} = 0$ we get Eqs. (4.10a) and (4.10b), respectively.

Mathematical Deductions from Some Rules Concerning High-Energy Total Cross Sections*

C. N. YANG†
Brookhaven National Laboratory, Upton, New York
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Mathematical implications of the Pomeranchuk rule and the Pomeranchuk-Okun rule are discussed.

IN 1956, Pomeranchuk[1] and Okun and Pomeranchuk[2] discussed a very interesting rule, which we shall call the Pomeranchuk-Okun rule. It states that at very high energies, in the forward direction, the exchange scattering amplitudes (such as charge exchange, strangeness exchange, etc.) are infinitesimal compared with the elastic amplitude. Two years later Pomeranchuk[3] discussed another very interesting rule, which we shall call the Pomeranchuk rule. It states that the total cross section in an $A + B$ collision is the same as that of $\bar{A} + B$ at very high energies. Both rules seem to have received increasing experimental support in recent years.

1. In this note we want to discuss the mathematical consequences of *each* of the two rules, when one takes into consideration the isotopic spin symmetry of the strong interactions. The results are valid only in so far as the effects of the electromagnetic and weak interactions are negligible. Higher symmetries are touched upon briefly in Sec. 5.

2. We shall use slightly generalized versions of the two rules: Each of the two colliding particles is supposed to be a coherent mixture of the various components of an isotopic spin multiplet (e.g., 70% proton plus 30% neutron). The same reasons for believing the original rules support this generalized version of the rules.

3. *Theorem 1*: The Pomeranchuk-Okun rule implies that at infinite energy the total cross section in a collision $A + B$ is independent of the total isotopic spin. In other words,

$$\sigma(A + B) = \sigma(A' + B')$$

if A and A', B and B' belong to the same isotopic multiplet.

Proof: Let $a = 1, 2, \cdots$, $b = 1, 2, \cdots$ denote the m-quantum numbers of the particles A and B, respectively. Let

$$\langle a', b' \,|\alpha|\, a, b\rangle \tag{1}$$

denote the forward scattering amplitude (times $4\pi\lambda$) from $A + B$ to $A' + B'$. Then the Pomeranchuk-Okun rules states that

$$\langle a', b' \,|\alpha|\, ab\rangle = \text{diagonal}.$$

The rule states in fact that (1) still holds if one changes the representations of the particles A by a unitary transformation U and that of B by a unitary transformation V:

$$\langle a', b' \,|UV\alpha V^{-1}U^{-1}|\, ab\rangle = \text{diagonal}. \tag{2}$$

It follows easily from (2) that α is a multiple of the unit matrix. Taking its imaginary part, one obtains the theorem.

4. In this section we shall discuss the consequences of the Pomeranchuk rule irrespective of the validity of the Pomeranchuk-Okun rule.

Theorem 2: The Pomeranchuk rule is equivalent to the rule that at ∞ energy, $\sigma_J = \sum_{J'} M_{JJ'}\bar{\sigma}_{J'}$ where

$$M_{JJ'} = (-1)^{2A+2B}(2J' + 1)\begin{Bmatrix} ABJ \\ ABJ' \end{Bmatrix},$$

A and B stand for the total isotopic spins of particles A and B (as well as for the particles themselves), the $\{\ \}$ for the $6J$ symbol,[4] and σ_J, $\bar{\sigma}_J$, respectively, for the total cross sections[5] with total isotopic spin J in the collisions $A + B$ and $A + \bar{B}$.

Proof: (a) Take the forward scattering amplitude matrix α of (1) and let

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† Permanent address: The Institute for Advanced Study, Princeton, New Jersey.

[1] I. Ia. Pomeranchuk, J. Exptl. Theoret. Phys. (U. S. S. R.) **30**, 423 (1956) [translation: Soviet Phys.—JETP **3**, 306 (1956)].

[2] L. B. Okun and I. Ia. Pomeranchuk, J. Exptl. Theoret. Phys. (U. S. S. R.) **30**, 424 (1956) [translation: Soviet Phys.—JETP **3**, 307 (1956)].

[3] I. Ia. Pomeranchuk, J. Exptl. Theoret. Phys. (U. S. S. R.) **34**, 725 (1958) [Translation; Soviet Phys.—JETP **7**, 499 (1958)].

[4] See, e.g., A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

[5] That $6J$ symbols are useful for discussions concerning crossing symmetry was pointed out by G. C. Wick, Brookhaven Lectures, 1960 (unpublished).

$$\beta = -\tfrac{1}{2}i(\alpha - \alpha^+). \quad (3)$$

β is thus the imaginary part of the forward scattering amplitude. Its diagonal elements are the total cross sections. We define the *corresponding* matrices $\bar{\alpha}$ and $\bar{\beta}$ for $A + \bar{B}$ collisions. The Pomeranchuk rule states that

$$\text{diagonal elements of } (\beta - \bar{\beta}) = 0. \quad (4)$$

Under a unitary transformation U on the states of A and a unitary transformation V on the states of B, the matrices β and $\bar{\beta}$ transform by:

$$\beta \to UV\beta V^{-1}U^{-1}, \qquad \bar{\beta} \to UV^*\bar{\beta}V^{*-1}U^{-1}.$$

Thus the generalized Pomerancuk rule states that diagonal element of

$$(UV\beta V^{-1}U^{-1} - UV^*\bar{\beta}V^{*-1}U^{-1}) = 0. \quad (5)$$

Since U is an arbitrary unitary matrix operating on the states of A, (5) is equivalent to

$$\langle ab\,|V\beta V^{-1} - V^*\bar{\beta}V^{*-1}|\,a'b\rangle = 0. \quad (6)$$

Since V is unitary, (6) is equivalent to

$$\langle ab\,|V\beta V^{-1}|\,a'b\rangle = \langle a'b\,|V\bar{\beta}V^{-1}|\,ab\rangle. \quad (7)$$

Since V is an arbitrary unitary matrix operating on the states of b, (7) is equivalent to

$$\langle ab\,|\beta|\,a'b'\rangle = \langle a'b\,|\bar{\beta}|\,ab'\rangle,$$

or to

$$\langle ab\,|\beta|\,a'b'\rangle = \langle ab'\,|\bar{\beta}|\,a'b\rangle. \quad (8)$$

(b) We can express β in terms of σ_J and Clebsch Gordon coefficients[4]

$$\langle ab\,|\beta|\,a'b'\rangle = \sum_{Jm} \langle ab\,|\,Jm\rangle\sigma_J\langle Jm\,|\,a'b'\rangle. \quad (9)$$

We can also express $\bar{\beta}$ in terms of $\bar{\sigma}_J$, Clebsch Gordon coefficients and the symbols[4] $\binom{J}{mm'}$:

$$\langle ab'\,|\bar{\beta}|\,a'b\rangle = \sum_{\substack{b''b'''\\ J'm'}} \binom{B}{b'b''}\binom{B}{bb'''} \times \langle ab''\,|\,J'M'\rangle\bar{\sigma}_{J'}\langle J'm'\,|\,a'b'''\rangle. \quad (10)$$

The occurrence of the symbols $\binom{J}{mm'}$ is due to the definition of $\bar{\beta}$ in which the rows and columns are labeled to correspond to the rows and columns of β.

(c) Substituting (9) and (10) into (8) one obtains, after some straightforward algebra, the relationship between σ_J and $\overline{\sigma_J}$, given by theorem 2.

We now discuss in detail the consequences of Theorem 2 for the following three cases:

(A) A and $\bar{A}$ do not belong to the same isotopic spin multiplet, and B and $\bar{B}$ do not belong to the same isotopic spin multiplet. In this case we have four sets of σ_J's: for $A + B$, $A + \bar{B}$, $\bar{A} + B$ and $\bar{A} + \bar{B}$. By repeated application of Theorem 2 one obtains

$$\sigma_J(A + B) = \sigma_J(\bar{A} + \bar{B}),$$

$$\sigma_J(A + \bar{B}) = \sigma_J(\bar{A} + B).$$

We have made use of the fact that the square matrix M multiplied by itself is unity, as can be easily verified from the properties of the $6J$ symbols. Furthermore, $\sigma_J(A + B)$ and $\sigma_J(A + \bar{B})$ are related by Theorem 2. There are thus altogether $2I + 1$ linearly independent total cross sections, where I is the smaller of the total isotopic spins of A and B.

(B) A and $\bar{A}$ do not belong to the same isotopic spin multiplet, B and $\bar{B}$ do. In this case, by definition,

$$\sigma_J(A + B) = \sigma_J(A + \bar{B}).$$

Thus, Theorem 2 shows that $\sigma_J(=\overline{\sigma_J})$ satisfies a set of linear homogeneous equations. These equations have been completely and explicitly solved.[6] In particular, the number of linearly independent total cross sections is

$$B + 1 \quad \text{for} \quad A \geq B,$$

$$A + \tfrac{1}{2} \quad \text{for} \quad A < B, \quad 2A = \text{odd},$$

$$A + 1 \quad \text{for} \quad A < B, \quad 2A = \text{even}.$$

It is obvious by repeated application of Theorem 2 that

$$\sigma_J(A + B) = \sigma_J(\bar{A} + B).$$

(C) A and $\bar{A}$ belong to the same isotopic spin multiplet. B and $\bar{B}$ belong to the same isotopic spin multiplet. In this case, the same conclusions as in case (B) obtain.

5. If one takes both the Pomeranchuk and the Pomeranchuk-Okun rule, one obtains, of course, trivially that all σ_J are the same for all J and for $A + B$, $\bar{A} + B$, etc.

6. The above considerations can clearly be made also for any compact group of symmetries of the strong interactions. To obtain a general solution, however, one must first have a proper definition of the $6J$ symbols, and one must know certain symmetry and summation properties of the $6J$ symbols. This is an unsolved problem.[7]

It is a pleasure to thank the members of the Physics Department of the Brookhaven National Laboratory for the hospitality extended to me during my visit.

[6] M. E. Rose and C. N. Yang, J. Math. Phys. **3**, 106 (1962).

[7] Cf. W. T. Sharp, Princeton University Thesis (1960) (unpublished).

Low-Energy Expansion of Scattering Phase Shifts for Long-Range Potentials*

BERTRAM R. LEVY AND JOSEPH B. KELLER
Courant Institute of Mathematical Sciences, New York University, New York, New York
(Received 22 June 1962)

Phase shifts can be used to describe the quantum mechanical scattering of a particle by a spherically symmetric potential. They are odd functions of the wave number k, which is proportional to the square root of the energy of the incident particle. For short-range potentials, they are analytic at $k = 0$ and can be expanded in odd powers of k. However for long-range potentials they are not analytic at $k = 0$ so they cannot be expanded in powers of k. Since electron–atom, atom–atom, proton–neutron, and multipole–multipole potentials are of long range, it is important to consider such potentials. A method is presented for determining the appropriate expansions around $k = 0$. The method is applied to potentials which are $O(r^{-\nu})$ as $r \to \infty$, and the phase shifts for any angular momentum are obtained up to and including the first nonanalytic term. For $L = 0$ and $3 < \nu < 4$ the next term is also obtained. The nonanalytic terms involve $\ln k$ and fractional powers of k. The results for $\nu = 4$ and the k dependence for $\nu = 2L + 3$ agree with those obtained in a different way by O'Malley, Spruch, and Rosenberg.

The method involves a function $\eta(r)$ whose asymptotic value $\eta(\infty)$ is the desired phase shift. A nonlinear first-order ordinary differential equation is derived for $\eta(r)$. This equation is solved by expansion and iteration methods. To expand the solution around $k = 0$, two simple theorems are proved concerning the asymptotic forms of certain integrals containing a parameter.

1. INTRODUCTION

In quantum mechanics the scattering of a particle by a spherically symmetric potential can be described in terms of phase shifts. Each phase shift is an odd function of the wave number k, which is proportional to the square root of the energy of the incident particle. For short-range potentials, the phase shifts are analytic at $k = 0$ so they can be expanded in odd powers of k. The first two coefficients in this expansion are related to the scattering length and the effective range of the potential, which are useful in describing low-energy scattering. For long-range potentials, however, the phase shifts are not analytic at $k = 0$, so they cannot be expanded in powers of k. Therefore we shall present a method for determining their appropriate expansions around $k = 0$, for long-range as well as short-range potentials. These expansions are of interest because the potential between a charged particle and a multipole and that between any two multipoles are long range. Thus, examples of long-range potentials are the van der Waals potential between two atoms, the polarization potential between an electron and an atom with a permanent or induced dipole moment, the neutron–proton, magnetic dipole–magnetic dipole interaction, etc.

Our work was stimulated by that of O'Malley, Spruch, and Rosenberg.[1] They realized, although they did not prove, that in principle, the Born expansion of the Lth phase shift η^L can be reexpanded for small k to yield the terms preceding k^{2L+1} in the expansion of η^L. Previous investigators had expected this method to give only the k dependence of these terms. Although the procedure is not very practical, they did use it to obtain the first term in certain cases. They also obtained several terms in the expansions of the phase shifts for an r^{-4} potential by solving the radial Schrödinger equation in terms of Mathieu functions and utilizing their known properties. We devised our method to obtain corresponding results for any long-range potential. O'Malley, Rosenberg, and Spruch[2] have used their results to treat low-energy scattering of electrons by hydrogen atoms.

The method begins with the introduction of a function $\eta(r)$ which may be called the phase shift as a function of r. It represents the phase shift due to a potential $V(r)$ truncated at r, i.e., $V(\rho) = 0$ for $\rho > r$. The desired phase shift is $\eta(\infty)$. The function $\eta(r)$ satisfies a nonlinear first-order ordinary differential equation which has occasionally been considered before. We derive it and then solve it in Sec. 2 by expanding $\eta(r)$ as a series in odd powers of k and determining the expansion coefficients, which are functions of r. For short-range potentials, all these coefficients have finite limits at $r = \infty$, and they yield the expansion of $\eta(\infty)$, which agrees with that obtained by the usual method as we show

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[1] T. O'Malley, L. Spruch, and L. Rosenberg, J. Math. Phys. 2, 491 (1961).

[2] T. O'Malley, L. Rosenberg, and L. Spruch, Phys. Rev. 125, 1300 (1962).

in Appendix I. However, for long-range potentials, at most a finite number of coefficients have finite limits at $r = \infty$ and the subsequent ones become infinite. In Sec. 3 the procedure for finding $\eta(\infty)$ is modified and the first non analytic term is obtained. The results are given in Eqs. (26)–(28). In Sec. 4 the next term in $\eta(\infty)$ is obtained for the r^{-4} potential and the result (33) for this case is shown to agree with that of O'Malley, Spruch, and Rosenberg.[1] In Secs. 2 to 4, only the case $L = 0$ is considered for simplicity. Corresponding results for any value of L are obtained in Sec. 5 and summarized in (67) to (70). Some theorems on the asymptotic evaluation of certain integrals, which are employed in the analysis, are stated and proved in Appendix II.

2. FORMULATION OF THE METHOD FOR L = 0

Let $r^{-1}u(r)$ denote the radial wave function, corresponding to angular momentum zero, for a particle in the presence of the spherically symmetric potential $\hbar^2V(r)/2\mu$. Here μ is the reduced mass of the particle and $\hbar$ is Planck's constant divided by 2π. Since $r^{-1}u$ satisfies the Schrödinger equation and is finite at $r = 0$, u satisfies the equations

$$u'' + [k^2 - V(r)]u = 0, \tag{1}$$

$$u(0) = 0. \tag{2}$$

The wave number k is related to the energy E of the particle by the relation $k^2 = 2\mu E/\hbar^2$.

To solve (1) and (2) we write $u(r)$ in terms of a phase function $\eta(r)$ and an amplitude $A(r)$ in the form

$$u(r) = A(r) \sin [kr + \eta(r)]. \tag{3}$$

Since we have introduced two new functions to express $u(r)$, we may impose some condition upon them and, therefore, we require

$$u'(r) = kA(r) \cos [kr + \eta(r)]. \tag{4}$$

Upon inserting (3) into (4) we obtain

$$A' \sin (kr + \eta) = -A\eta' \cos (kr + \eta). \tag{5}$$

We now insert (3) into (1) and use (5) to express A' in terms of A. In this way we can eliminate A and obtain the following equation for $\eta(r)$

$$\eta'(r) = -k^{-1}V(r) \sin^2 [kr + \eta(r)]. \tag{6}$$

In order that $u(r)$ satisfy (2), we find

$$\eta(0) = 0. \tag{7}$$

To solve (6) and (7) we represent $\eta(r)$ as a series in odd powers of k with coefficients $\eta_i(r)$ that are to be determined:

$$\eta(r) = k \sum_{i=0}^{\infty} k^{2i}\eta_i(r). \tag{8}$$

Upon substituting (8) into (6), expanding the sine function in a power series and equating the coefficients of like powers of k, we obtain a recursive system of differential equations for the $\eta_i(r)$. The first three of them are

$$\eta_0' = -V(r)(r + \eta_0)^2, \qquad \eta_0(0) = 0 \tag{9}$$

$$\eta_1' = -2V(r)(r + \eta_0)\eta_1 + \tfrac{1}{3}V(r)(r + \eta_0)^4, \qquad \eta_1(0) = 0 \tag{10}$$

$$\eta_2' = -2V(r)(r + \eta_0)\eta_2 - V(r)\eta_1 + \tfrac{1}{3}4V(r)(r + \eta_0)\eta_1 - \tfrac{2}{45}V(r)(r + \eta_0)^6, \qquad \eta_2(0) = 0. \tag{11}$$

From (7) we see that for each j, $\eta_j(0) = 0$. We assume that $h_0(r)$ is finite for all r.

Once $\eta_0(r)$, the solution of (9), has been found, the remaining $\eta_j(r)$ can be determined explicitly since they are solutions of first-order linear differential equations of the form (10) or (11). Upon evaluating them at $r = \infty$ we obtain

$$\eta_1(\infty) = \tfrac{1}{3}\int_0^{\infty} \exp\left[-2\int_r^{\infty} V(x)(x + \eta_0)^2\,dx\right] \times V(r)(r + \eta_0)^4\,dr, \tag{12}$$

$$\eta_2(\infty) = -\int_0^{\infty} \exp\left[-2\int_r^{\infty} V(x)(x + \eta_0)^2\,dx\right] \times V(r)[\eta_1 - \tfrac{4}{3}(r + \eta_0)\eta_1 + \tfrac{2}{45}(r + \eta_0)^6]\,dr. \tag{13}$$

The integrals in (12) and (13), and the corresponding ones for higher values of j, all converge for a short-range potential. By a short-range potential we mean one for which $V(r) = O(r^{-\nu})$ as $r \to \infty$ for every positive value of ν. Thus, for such potentials (8) yields

$$\eta(\infty) = k \sum_{i=0}^{\infty} k^{2i}\eta_i(\infty). \tag{14}$$

In Appendix I it is shown that the first two terms in (14) agree with those of the usual effective range theory. The scattering length A and the effective range r_0 are shown to be given by

$$A = -\eta_0(\infty), \tag{15}$$

$$r_0 = -\tfrac{2}{3}\eta_0(\infty) - 2\eta_1(\infty)/\eta_0^2(\infty). \tag{16}$$

3. LONG-RANGE POTENTIALS WITH L = 0

For a potential which is not short range, the integrals representing most of the $\eta_j(r)$ fail to con-

verge as $r \to \infty$. To see this, let us consider a long-range potential that is asymptotically of the form

$$V(r) = V_0 r^{-\nu} + O(r^{-\nu-1}) \quad \text{as} \quad r \to \infty. \tag{17}$$

Here $\nu > 3$ is a real number and V_0 is a positive or negative constant. From the recursive system of differential equations for the $\eta_i(r)$, we find that

$$\eta_i'(r) \sim (-1)^{i+1} \frac{(2r)^{2i+2}}{2(2i+2)!} V(r) \quad \text{as} \quad r \to \infty. \tag{18}$$

Thus $\eta_i(\infty)$ will be finite if $2i + 2 - \nu < -1$. Let m denote the largest value of i for which this inequality is satisfied. Then m is the largest integer which is less than $(\nu - 3)/2$, which we denote by the brace symbol

$$m = \{(\nu - 3)/2\}. \tag{19}$$

If $i \leq m$, $\eta_i(\infty)$ is finite, while if $i > m$, $\eta_i(\infty)$ is infinite. Therefore in order to determine $\eta(\infty)$ we modify the preceding method in the following manner.

For a long range potential satisfying (17) we introduce a new unknown function $\beta(r, k)$ by writing

$$\eta(r) = k \sum_{i=0}^{m} k^{2i} \eta_i(r) + k\beta(r, k). \tag{20}$$

Here m is given by (19) and the $\eta_i(r)$ are given by the preceding construction. To determine β we insert (20) into (6) and (7) and obtain

$$\beta' = -k^{-2} V(r) \sin^2 (kr + \eta) - \sum_{i=0}^{m} k^{2i} \eta_i', \qquad \beta(0, k) = 0. \tag{21}$$

From the fact that $\eta_{m+1}(r)$ diverges as $r \to \infty$, it is clear that the leading term in the asymptotic expansion of $\beta(\infty, k)$ for small k comes from the neighborhood of $r = \infty$. Consequently, in (21) we shall retain only the most singular part of $\eta_i'(r)$ at $r = \infty$ and, omit η in the sine function. Then upon integrating (21) and denoting the result by $B(r, k)$ we obtain

$$B(r, k) = -k^{-2} \int_0^r V(r) \times \left[\sin^2 kr - \frac{1}{2} \sum_{i=0}^{m} \frac{(-1)^i (2kr)^{2i+2}}{(2i+2)!} \right] dr. \tag{22}$$

The preceding considerations indicate why the leading term in the expansion of $\beta(\infty, k)$ is the same as that of $B(\infty, k)$. We shall prove that this is so far the special case of $\nu = 4$ in Appendix III. A similar proof can presumably be constructed for any value of ν, but we shall not consider it.

The integrand in (22) is $O(r^{2m+2-\nu})$ as $r \to \infty$ since $m \geq 0$ so the integral converges as $r \to \infty$, as a consequence of the definition (19) of m and of the condition $\nu > 3$. The asymptotic form of $B(\infty, k)$ can be obtained from (22) by applying Theorem 1 of Appendix II when ν is not an odd integer. This theorem shows that the asymptotic form of $B(\infty, k)$ is obtained by inserting the asymptotic form of $V(r)$ into (22) with the result

$$\beta(\infty, k) \sim B(\infty, k) \sim -V_0 |k|^{\nu-3} \times \int_0^\infty r^{-\nu} \left[\sin^2 r - \frac{1}{2} \sum_{i=0}^{m} \frac{(-1)^i (2r)^{2i+2}}{(2i+2)!} \right] dr, \qquad 3 < \nu \neq 5, 7 \cdots. \tag{23}$$

At the origin the integrand is $O(r^{2m+4-\nu})$ so the integral is convergent there since ν is not an odd integer. When ν is an odd integer, then $m = (\nu - 5)/2$ and we find from Theorem 2 of Appendix II that $B(\infty, k)$ has the following asymptotic form

$$\beta(\infty, k) \sim B(\infty, k) \sim \frac{V_0 (-1)^{(\nu+1)/2}}{(\nu - 1)!} 2^{\nu-2} |k|^{\nu-3} \ln |k| \qquad \nu = 5, 7 \cdots. \tag{24}$$

If ν lies in the interval $3 < \nu < 4$ we can obtain an additional term in the expansion of $\beta(\infty, k)$ beyond that given in (23). We do so at the end of Appendix III by expanding $B(\infty, k)$ to two terms and proving that for $3\frac{1}{2} < \nu < 4$, $\beta(\infty, k) - B(\infty, k) = 0(k^2)$. Since this difference vanishes to a higher order than both of these terms they are both valid and the result is

$$\beta(\infty, k) \sim B(\infty, k) \sim -V_0 |k|^{\nu-3} \times \int_0^\infty \frac{\sin^2 r - r^2}{r^\nu} dr + \eta_0(\infty) |k|^{\nu-2} \times \int_0^\infty \frac{\sin 2r - 2r}{r^\nu} dr, \qquad 3 < \nu < 4. \tag{25}$$

Presumably, a similar proof of the validity of the second term could be given for $3 < \nu \leq 3\frac{1}{2}$, but we have not considered it.

Upon inserting the results (23), (24), or (25) into (20) after letting $r = \infty$, we obtain the expansion of $\eta(\infty)$ up to and including the first nonanalytic term for all values of $\nu > 3$. When $3 < \nu < 4$ we also have an additional term. The results for $\eta(\infty)$ are:

$$\eta(\infty) \sim k \sum_{i=0}^{m} k^{2i} \eta_i(\infty) - V_0 k |k|^{\nu-3} \times \int_0^\infty r^{-\nu} \left[\sin^2 r - \frac{1}{2} \sum_{i=0}^{m} \frac{(-1)^i (2r)^{2i+2}}{(2i+2)!} \right] dr, \qquad 3 < \nu \neq 5, 7, \cdots. \tag{26}$$

$$\eta(\infty) \sim k \sum_{i=0}^{(\nu-5)/2} k^{2i}\eta_i(\infty) + \frac{V_0(-2)^{(\nu+1)/2}}{(\nu-1)!} k\,|k|^{\nu-3} \ln|k|, \quad \nu = 5, 7, \cdots \tag{27}$$

$$\eta(\infty) \sim k\eta_0(\infty) - V_0 k\,|k|^{\nu-3} \int_0^\infty r^{-\nu}(\sin^2 r - r^2)\,dr + \eta_0(\infty) k\,|k|^{\nu-2} \int_0^\infty r^{-\nu}(\sin 2r - 2r)\,dr, \quad 3 < \nu < 4. \tag{28}$$

In (26) m is defined by (19). In the next section we shall obtain another term when $\nu = 4$, thereby illustrating a procedure that can be used for any value of ν.

4. THE R^{-4} POTENTIAL WITH L = 0

In the previous section we introduced $\beta(r, k)$ in (20) and obtained Eq. (21), which it satisfies. We indicated that the leading term in $\beta(\infty, k)$ is the same as that of $B(\infty, k)$ defined by (22) and we computed the latter. Now we shall solve (21) by iterations and show that the leading term in $\beta(\infty, k)$ is indeed that which we previously obtained. We shall also calculate the next term in $\beta(\infty, k)$. These calculations will be done for the special case $\nu = 4$ because the labor is then not too great.

For $\nu = 4$, (19) shows that $m = 0$, so (20) and (21) become

$$\eta(r) = k\eta_0(r) + k\beta(r, k), \tag{29}$$

$$\beta' = -k^{-2}V(r)[\sin^2(kr + k\eta_0 + k\beta) - k^2(r + \eta_0)^2], \quad \beta(0) = 0. \tag{30}$$

We solve (30) by iterations, defining the nth approximation β_n by setting $\beta_0 = 0$ and

$$\beta_n = -k^{-2} \int_0^r V(t)[\sin^2(kt + k\eta_0 + k\beta_{n-1}) - k^2(t + \eta_0)^2]\,dt. \tag{31}$$

In Appendix III we show that for $n = 1, 2, \cdots$ we have, uniformly in r,

$$\beta_n(r, k) = O(k) \tag{32}$$

$$\beta_{n+1}(r, k) - \beta_n(r, k) = O(k^2). \tag{33}$$

Thus the phase shift can be obtained up to terms of order k^2 from β_1. In Appendix III we show that

$$\beta_1(\infty, k) = \tfrac{1}{3}|k|\,V_0\pi - \tfrac{4}{3}\eta_0(\infty)V_0k^2 \ln|k| + O(k^2). \tag{34}$$

The phase shift is then

$$\eta(\infty) = k\eta_0(\infty) + \tfrac{1}{3}k\,|k|\,V_0\pi - \tfrac{4}{3}\eta_0(\infty)V_0k^3 \ln|k| + O(k^3). \tag{35}$$

This result agrees with that of O'Malley, Spruch, and Rosenberg,[1] who also determined the k^3 term.

5. PHASE SHIFTS FOR L > 0

We shall now consider the phase shift for any value of $L > 0$. We let $r^{-1}u(r)$ denote the radial wave function, corresponding to angular momentum L. Then u satisfies the equations

$$u'' + [k^2 - V(r) - L(L+1)/r^2]u = 0, \tag{36}$$

$$u(0) = 0. \tag{37}$$

In order to obtain an equation for the phase shift as a function of r, we introduce the functions

$$\varphi(r) = krj_L(kr) = (\pi kr/2)^{1/2}J_{L+1/2}(kr), \tag{38}$$

and

$$\psi(r) = krn_L(kr) = (\pi kr/2)^{1/2}N_{L+1/2}(kr). \tag{39}$$

The functions j_L and n_L are spherical Bessel functions and the functions $\varphi(r)$ and $\psi(r)$ are solutions of (36) with $V(r) \equiv 0$.

We introduce the phase shift $\eta(r)$ by writing the solution of (36) and (37) as

$$u(r) = A(r)[\varphi(r) - \psi(r)\tan\eta(r)]. \tag{40}$$

The desired phase shift is as before $\eta(\infty)$. As before we have introduced two new functions $A(r)$ and $\eta(r)$. We now impose the condition that

$$A'(r)[\varphi - \psi\tan\eta] = A\psi\,\eta'\sec^2\eta. \tag{41}$$

Then,

$$u' = A[\varphi' - \psi'\tan\eta]. \tag{42}$$

Differentiating once more we find

$$u'' = A'[\varphi' - \psi'\tan\eta] + A[\varphi'' - \psi''\tan\eta] - A\,\eta'\psi'\sec^2\eta. \tag{43}$$

We next substitute (40) and (43) into (36). Upon using the fact that φ and ψ satisfy (36) with $V(r) = 0$, we find that

$$A'[\varphi' - \psi'\tan\eta] - A\,\eta'\psi'\sec^2\eta - VA(\varphi - \psi\tan\eta) = 0. \tag{44}$$

We now eliminate A' between (44) and (41) and use the fact that the Wronskian $\varphi'\psi - \psi'\varphi$ has the value $-k$, to obtain

$$\eta'\sec^2\eta = -k^{-1}V(r)\{\varphi - \psi\tan\eta\}^2. \tag{45}$$

Upon expressing φ and ψ in terms of spherical Bessel functions by means of (38) and (39), we find

$$(d/dr)\tan\eta = -kr^2V(r)\{j_L(kr) - n_L(kr)\tan\eta\}^2. \quad (46)$$

In order to satisfy the initial condition (37), we note that since $j_L(kr)$ vanishes at the origin we must have

$$\eta(0) = 0. \quad (47)$$

Equations (46) and (47) are the desired equations for the phase shift $\eta(r)$ or for $\tan\eta(r)$.

In order to analyze (46) for the case of short-range potentials, we denote $\tan\eta(r)$ by $\chi(r)$ and set

$$\chi(r) = k^{2L+1}\sum_{j=0}^{\infty} k^{2j}\chi_j(r). \quad (48)$$

Upon substituting (48) into (46) for $\tan\eta$, expanding j_L and n_L in power series, and equating the coefficients of like powers of k, we obtain a recursive system of differential equations for the $\chi_j(r)$. The first two of them are

$$\chi_0' = -V(r)(c_0r^{L+1} - \chi_0\, d_0r^{-L})^2, \quad \chi_0(0) = 0, \quad (49)$$

$$\chi_1' = -2V(r)(c_0r^{L+2} - \chi_0\, d_0r^{-L+1}) \times (c_1r^{L+2} - \chi_0\, d_1r^{-L+1} - \chi_1\, d_0r^{-L-1}), \quad \chi_1(0) = 0. \quad (50)$$

Here

$$c_0 = \frac{2^LL!}{(2L+1)!}, \qquad d_0 = -\frac{1}{2^L}\frac{\Gamma(2L+1)}{\Gamma(L+1)},$$
$$c_1 = -\frac{2^L(L+1)!}{(2L+3)!}, \qquad d_1 = -\frac{1}{2^L}\frac{\Gamma(2L-1)}{\Gamma(L)}. \quad (51)$$

Just as in the case for $L = 0$, after $\chi_0(r)$ is determined by solving (49), the remaining χ_j are obtained by solving simple, linear, first-order ordinary differential equations. Since $V(r) = O(r^{-\nu})$ for every ν, $\chi_j(\infty)$ will exist.

In the case of long-range potentials, $\chi_j(\infty)$ will not exist for j sufficiently large. Since

$$\chi_j' = O[V(r)r^{2(L+1+j)}], \quad \text{as} \quad r \to \infty, \quad (52)$$

it is clear that if $V(r) \sim V_0r^{-\nu}$ as $r \to \infty$, then $\chi_j(\infty)$ will exist only if

$$2j < \nu - 2L - 3. \quad (53)$$

As before, when (53) is violated we must proceed by introducing a new expansion. Let m be the largest value of j for which (53) holds. Then we write

$$\chi = k^{2L+1}\sum_{j=0}^{m} k^{2j}\chi_j + \beta. \quad (54)$$

Then β satisfies

$$\beta' = -kr^2V(r)\{j_L(kr) - \chi n_L(kr)\}^2 - k^{2L+1}\sum_{j=0}^{m} k^{2j}\chi_j'. \quad (55)$$

In order to obtain the leading term in β we drop χ on the right-hand side of (55) and replace χ_j' by its most singular part as $r \to \infty$. In order to do, this we write the power-series expansion for $[j_L(kr)]^2$ in the following form:

$$[j_L(kr)]^2 = (kr)^{2L}\sum_{j=0}^{\infty} f_j(kr)^{2j}. \quad (56)$$

Here

$$f_j = \sum_{k=0}^{j} c_kc_{j-k}, \quad (57)$$

$$c_j = \frac{2^L(-1)^j(L+j)!}{j!(2L+2j+1)!}. \quad (58)$$

From (49), (50), and similar equations for the higher χ_j, we find

$$\chi_j' \sim -r^{2L+2}V(r)f_jr^{2j}, \quad \text{as} \quad r \to \infty. \quad (59)$$

We now insert (59) into (55), drop χ on the right-hand side, and integrate. The resulting function we denote by $B(r, k)$ and, as before, we expect that $\beta(r, k) \sim B(r, k)$, where B is defined by

$$B(r, k) = -k\int_0^r r^2V(r) \times \left\{[j_L(kr)]^2 - (kr)^{2L}\sum_{j=0}^{m} f_j(kr)^{2j}\right\} dr. \quad (60)$$

We can apply Theorem I of Appendix II when $2m > \nu - 2L - 5$. From the definition of m, this inequality is satisfied unless ν is an odd integer. Thus except for such ν, Theorem I applied to (60) yields

$$B(\infty, k) \sim -V_0k^{-1}|k|^{\nu-1}\int_0^{\infty} r^{2-\nu} \times \left\{[j_L(r)]^2 - r^{2L}\sum_{j=0}^{m} f_jr^{2j}\right\} dr, \quad \nu \neq 5, 7 \cdots. \quad (61)$$

When $2m = \nu - 2L - 5$, which occurs when ν is an odd integer, Theorem II of Appendix II applied to (60) yields

$$B(\infty, k) \sim V_0k^{-1}f_{(\nu-3)/2-L}|k|^{\nu-1}\ln|k|, \quad \nu = 5, 7 \cdots. \quad (62)$$

In the case when $3 < \nu \leq 2L + 3$, so that there is no value of $j \geq 0$ satisfying (53), then (61) is still valid for $\nu < 2L + 3$ if the sum involving

f_i on the right is dropped. Similarly, for $\nu = 2L + 3$, (62) is valid if we replace f_{m+1} by f_0. In the case when $\nu < 2L + 3$, the integral appearing in (61) can be explicitly evaluated. We first express j_L in terms of cylindrical Bessel functions by means of (38), obtaining

$$B(\infty, k) \sim -\tfrac{1}{2}\pi V_0 k^{-1} |k|^{\nu-1} \int_0^\infty r^{1-\nu}[J_{L+1/2}(r)]^2 \, dr. \tag{63}$$

This is just the expression for $\tan \eta(\infty)$ given by the first Born approximation.

The integral in (63) is a known Mellin transform.[3] When this integral is evaluated we obtain

$$B(\infty, k) \sim -\tfrac{1}{2}\pi V_0 k^{-1} |k|^{\nu-1} \times \frac{2^{1-\nu}\Gamma(\nu-1)\Gamma(L+\frac{3}{2}-\nu/2)}{\Gamma^2(\frac{1}{2}\nu)\Gamma(L+\frac{1}{2}+\frac{1}{2}\nu)}. \tag{64}$$

In particular, if $\nu = 4$, (64) holds for all $L > 0$ and yields, with $V_0 = -\beta^2$,

$$B(\infty, k) \sim \frac{\pi\beta^2 k^{-1}|k|^3}{8(L+\frac{3}{2})(L+\frac{1}{2})(L-\frac{1}{2})}. \tag{65}$$

This is the same as Eq. (5.9) of O'Malley, Spruch, and Rosenberg.[1]

Let us now summarize the results of this section, which are valid for $L \geq 0$. For a short-range potential, we have from (48)

$$\tan \eta(\infty) = k^{2L+1} \sum_{i=0}^{\infty} k^{2i}\chi_i(\infty). \tag{66}$$

The χ_i are determined by solving the system of recursive equations, of which (49) and (50) are the first two members. For a long-range potential, $V(r) \sim V_0 r^{-\nu}$ as $r \to \infty$, we have from (54) and (64), (62), or (61)

$$\tan \eta(\infty) \sim -\tfrac{1}{2}\pi V_0 k |k|^{\nu-3} \times \frac{2^{1-\nu}\Gamma(\nu-1)\Gamma(L+\frac{3}{2}-\frac{1}{2}\nu)}{\Gamma^2(\frac{1}{2}\nu)\Gamma(L+\frac{1}{2}+\frac{1}{2}\nu)}, \quad 3 < \nu < 2L+3, \tag{67}$$

$$\tan \eta(\infty) \sim \frac{V_0 k |k|^{2L}}{[1\cdot 3\cdot 5 \cdots (2L+1)]^2} \ln |k|, \quad \nu = 2L+3, \tag{68}$$

$$\tan \eta(\infty) \sim k^{2L+1} \sum_{i=0}^{m} k^{2i}\chi_i(\infty) - V_0 k |k|^{\nu-3} \times \int_0^\infty r^{2-\nu}\left\{[j_L(r)]^2 - r^{2L}\sum_{i=0}^{m} f_i r^{2i}\right\} dr, \quad 2L+3 < \nu \neq 5, 7, \cdots, \tag{69}$$

[3] Bateman Manuscript Project, *Tables of Integral Transforms*, edited by A. Erdelyi, (MacGraw-Hill Book Company, Inc., New York, 1954), pp. 1, 331.

$$\tan \eta(\infty) \sim k^{2L+1} \sum_{i=0}^{(\nu-5)/2} k^{2i}\chi_i(\infty) + V_0 f_{(\nu-3)/2-L} k |k|^{\nu-3} \ln |k| \quad 2L+3 < \nu = 5, 7, \cdots. \tag{70}$$

Both (69) and (70) are valid when $\nu < 2L + 3$ or $\nu \leq 2L + 3$, respectively, but then the sums must be omitted, and they reduce to (67) and (68), respectively. For $L = 0$ the above results reduce to (26) and (27). For certain potentials (e.g. repulsive ones), (67) probably holds for $2 < \nu < 3$ and (68) for $\nu = 3$ and $L = 0$.

APPENDIX I. RELATION WITH EFFECTIVE-RANGE THEORY

In the usual effective-range terminology, the phase shift $\eta(\infty)$ is given by

$$k \cot \eta(\infty) = -1/A + \tfrac{1}{2}k^2 r_0 + O(k^3). \tag{A1}$$

If we use our result (14) for $\eta(\infty)$ and expand $k \cot \eta(\infty)$ in powers of k, we obtain

$$k \cot \eta(\infty) = \frac{1}{\eta_0(\infty)} - k^2\left[\frac{\eta_0(\infty)}{3} + \frac{\eta_1(\infty)}{\eta_0^2(\infty)}\right] + O(k^3). \tag{A2}$$

Upon comparing (A1) with (A2) we obtain the expressions (15) and (16) for A and r_0 in terms of $\eta_0(\infty)$ and $\eta_1(\infty)$. The result (16) differs in form from the usual expression for r_0, which is

$$r_0 = 2\int_0^\infty (v_0^2 - u_0^2)\, dr. \tag{A3}$$

Here $u_0(r)$ is the solution of (1) and (2) for $k = 0$ normalized so that

$$u_0(r) \sim 1 - A^{-1}r, \quad \text{as} \quad r \to \infty. \tag{A4}$$

The function $v_0(r)$ is defined by

$$v_0(r) = 1 - A^{-1}r. \tag{A5}$$

We shall now compute $u_0(r)$, insert it into (A3), and show that the result agrees with (16).

To this end we see from (18) that $\eta(r) = k\eta_0(r) + O(k^2)$. Upon using this result in (3) we may write $u_0(r)$ as

$$u_0(r) = kA_0(r)[r + \eta_0(r)]. \tag{A6}$$

Here $kA_0(r)$ denotes the limit of $A(r)$ at $k = 0$. From (5) we find that A_0 satisfies

$$A_0'[r + \eta_0] = -A_0\eta_0'. \tag{A7}$$

The solution of (A7) is

$$A_0(r) = a \exp\left\{-\int_r^\infty V(x)[x + \eta_0(x)]\, dx\right\}. \quad \text{(A8)}$$

The integration constant a is determined by the condition (A4). Then (A6) and (A8) yield

$$u_0(r) = -A^{-1}[r + \eta_0(r)] \times \exp\left\{-\int_r^\infty V(x)[x + \eta_0(x)]\, dx\right\}. \quad \text{(A9)}$$

Now (A3) becomes

$$r_0 = 2\int_0^\infty \left\{(1 - A^{-1}r)^2 - A^{-2}(r + \eta_0)^2 \times \exp\left[-2\int_r^\infty V(x)(x + \eta_0)\, dx\right]\right\} dr. \quad \text{(A10)}$$

In order to demonstrate the identity of (A10) and (16), let us consider the integral $I(M)$ defined by

$$I(M) = -\int_0^M V(x)(x + \eta_0)^4 \times \exp\left[-2\int_x^\infty V(r)(r + \eta_0)\, dr\right] dx. \quad \text{(A11)}$$

We note from (12) that $I(\infty) = -3\eta_1(\infty)$. Now we rewrite (A11) as

$$I(M) = -\frac{1}{2}\int_0^M (x + \eta_0)^3 \frac{d}{dx} \times \exp\left[-2\int_x^\infty V(r)(r + \eta_0)\, dr\right] dx \quad \text{(A12)}$$

Upon integrating by parts and using (9), we obtain from (A12),

$$I(M) = [M + \eta_0(M)]^3 \times \exp\left[-2\int_M^\infty V(r)(r + \eta_0)\, dr\right] - 3\int_0^M (x + \eta_0)^2 \times \exp\left[-2\int_x^\infty V(r)(r + \eta_0)\, dr\right] dx. \quad \text{(A13)}$$

Upon multiplying (A13) by $1/3\eta_0^2(\infty)$, and subtracting $\eta_0(\infty)/3$, it becomes

$$\frac{I(M)}{3\eta_0^2(\infty)} - \frac{\eta_0(\infty)}{3} = \int_0^M \left\{\left(1 + \frac{x}{\eta_0(\infty)}\right)^2 - \frac{(x + \eta_0)^2}{\eta_0^2(\infty)} \times \exp\left[-2\int_x^\infty V(r)(r + \eta_0)\, dr\right]\right\} dx + \delta. \quad \text{(A14)}$$

Here δ is given by

$$\delta = \frac{1}{3\eta_0^2(\infty)}[M + \eta_0(M)]^3 \times \exp\left[-2\int_M^\infty V(r)(r + \eta_0)\, dr\right] - \frac{\eta_0(\infty)}{3} - \int_0^M \left(1 + \frac{x}{\eta_0(\infty)}\right)^2 dx \quad \text{(A15)}$$

From (A15) we find, after performing the integration, that $\delta \to 0$ as $M \to \infty$. Then when $M \to \infty$, the right side of (A14) becomes one-half the right side of (A10) and the left side of (A14) becomes one-half the right side of (16). Thus, (16) and (A10) yield the same value of r_0.

APPENDIX II, ASYMPTOTIC EVALUATION OF TWO INTEGRALS

We wish to asymptotically, evaluate for small k, the function $B(\infty, k)$, represented by an integral in (22). This can be accomplished by means of two general theorems concerning such integrals which we shall now state and prove.

Theorem I. Let $I(k)$ be defined by

$$I(k) = \int_0^\infty V(r)f(kr)\, dr. \quad \text{(A16)}$$

Here $V(r)$ and $f(r)$ are regular and satisfy the following conditions

$$V(r) \sim V_0 r^{-\nu} \quad \text{as} \quad r \to \infty,$$
$$f(r) = O(r^{2m+2}) \quad \text{as} \quad r \to \infty,$$
$$f(r) = O(r^{2m+4}) \quad \text{as} \quad r \to 0.$$

The constants ν and m satisfy the relations

$$3 > \nu - 2m - 2 > 1, \qquad \nu > 0,\ m \geq 0$$

Then, for $k > 0$,

$$I(k) \sim V_0 |k|^{\nu-1} \int_0^\infty r^{-\nu} f(r)\, dr \quad \text{as} \quad k \to 0. \quad \text{(A17)}$$

If V and f satisfy the above conditions for $r \to -\infty$, then (A17) holds for $k < 0$.

Theorem II. Let $I(k)$ be defined by (A16) with $V(r)$ and $f(r)$ regular, and satisfying

$$V(r) \sim V_0 r^{-\nu}, \quad \text{as} \quad r \to \infty,$$
$$f(r) = O(r^{\nu-3}), \quad \text{as} \quad r \to \infty,$$
$$f(r) \sim f_0 r^{\nu-1}, \quad \text{as} \quad r \to 0.$$

Then for $k > 0$, $\nu > 0$

$$I(k) \sim -V_0 f_0 |k|^{\nu-1} \ln |k| \quad \text{as} \quad k \to 0. \quad \text{(A18)}$$

If V and f satisfy the above conditions for $r \to -\infty$, then (A18) holds for $k < 0$.

To prove Theorem I we introduce a function $\omega(k)$ with the properties that $\omega(k) \to \infty$ and $k\omega(k) \to 0$ as $k \to 0$. Then we split $I(k)$ into two integrals:

$$I_1 = \int_\omega^\infty V(r)f(kr)\,dr,$$

$$I_2 = \int_0^\omega V(r)f(kr)\,dr.$$

We also write $V(r)$ in terms of a function $\epsilon(r)$ in the form

$$V(r) = V_0 r^{-\nu}[1 + \epsilon(r)].$$

From the behavior of $V(r)$ at infinity it follows that $\epsilon(r) \to 0$ as $r \to \infty$. We may now write I_1 as a sum

$$I_1 = V_0 \int_\omega^\infty r^{-\nu} f(kr)\,dr + V_0 \int_\omega^\infty \epsilon(r) r^{-\nu} f(kr)\,dr. \quad \text{(A19)}$$

We now define $\bar{\epsilon}(\omega) = \sup_{r \geq \omega} \epsilon(r)$. Then the last integral above satisfies

$$\left| \int_\omega^\infty \epsilon(r) r^{-\nu} f(kr)\,dr \right| < \bar{\epsilon}(\omega) \int_\omega^\infty |r^{-\nu} f(kr)|\,dr$$

$$= \bar{\epsilon}(\omega)\,|k|^{\nu-1} \int_{k\omega}^\infty |r^{-\nu} f(r)|\,dr.$$

The last expression shows that the second integral in (A19) is of order $\bar{\epsilon}(\omega)\,|k|^{\nu-1}$.

To analyze the first integral in (A19), we introduce kr as a new integration variable and obtain

$$\int_\omega^\infty r^{-\nu} f(kr)\,dr = |k|^{\nu-1} \int_{k\omega}^\infty x^{-\nu} f(x)\,dx = |k|^{\nu-1} \times \left(\int_0^\infty x^{-\nu} f(x)\,dx + 0(k\omega) \right). \quad \text{(A20)}$$

From (A20) and (A19) we obtain

$$I_1 = V_0\,|k|^{\nu-1} \int_0^\infty r^{-\nu} f(r)\,dr + o(k^{\nu-1}). \quad \text{(A21)}$$

To analyze I_2 we utilize the mean-value theorem to conclude that

$$I_2 = O[\omega(k\omega)^{2m+4}]. \quad \text{(A22)}$$

Let us now set $\omega(k) = k^{-\alpha}$ where $\alpha < 1 - \nu/(2m+5)$. Then $0 < \alpha < 1$ so $\omega(k) \to \infty$ and $k\omega(k) \to 0$ as $k \to 0$. With this choice of $\omega(k)$, (A22) yields

$$I_2 = o(k^{\nu-1}). \quad \text{(A23)}$$

Upon combining (A21) and (A23) we obtain (A17), thus proving the theorem. The same proof applies when $k < 0$ if V and f satisfy the hypotheses as $r \to -\infty$.

In order to prove Theorem II we introduce the functions $\omega(k)$ and $\epsilon(r)$ and the integrals I_1 and I_2 as in the proof of Theorem I. We then find

$$I_1 = V_0\,|k|^{\nu-1} \left\{ \int_{k\omega}^\infty r^{-\nu} f(r)\,dr + \bar{\epsilon}(\omega) O\left(\int_{k\omega}^\infty |r^{-\nu} f(r)|\,dr \right) \right\}. \quad \text{(A24)}$$

We now introduce a constant $M > 0$ and write

$$\int_{k\omega}^\infty r^{-\nu} f(r)\,dr = \int_{k\omega}^M r^{-\nu} f(r)\,dr + O(1).$$

Upon making use of the behavior of f at the origin we find

$$\int_{k\omega}^\infty r^{-\nu} f(r)\,dr = -f_0 \ln |k\omega| + O(1).$$

A similar analysis holds for the order term in (A24). Thus (A24) becomes

$$I_1 = -V_0 f_0\,|k|^{\nu-1} \ln |k\omega| + \bar{\epsilon}(\omega)\,|k|^{\nu-1}\,O[\ln |k\omega|]. \quad \text{(A25)}$$

In order to analyze I_2 we use the asymptotic form of f at the origin assuming that $f(r) - V_0 r^{\nu-1} = O(r^\nu)$. Then from the mean-value theorem we obtain

$$I_2 = f_0\,|k|^{\nu-1} \int_0^\omega V(r) r^{\nu-1}\,dr + O[\omega(k\omega)^\nu]. \quad \text{(A26)}$$

Upon writing the integral in (A26) as the sum of two integrals; the first taken between the limits 0 and M, the second between the limits M and ω, and introducing the asymptotic form of V in the second integral we find

$$I_2 = V_0 f_0\,|k|^{\nu-1} \ln \omega + O(|k|^{\nu-1}) + O[\omega(k\omega)^\nu]. \quad \text{(A27)}$$

If we now set $\omega = |k|^{-\alpha}$, where $0 < \alpha < 1/(\nu+1)$, we find that (A25) and (A26) may be combined to yield (A18), thus proving Theorem II.

APPENDIX III. ASYMPTOTIC ESTIMATES OF THE ITERATES

We shall now prove (32) and (33) of Sec. 4 by induction. First we apply the mean-value theorem to the integrand of (31) for $n = 1$ and obtain

$$\beta_1(r) = \frac{k^2}{3} \int_0^r V(t)(t + \eta_0)^4 \cos\,[2k\theta(t)(t + \eta_0)]\,dt, \quad 0 < \theta(t) < 1. \quad \text{(A28)}$$

Next we define the difference $\Delta_n(r, k) = \beta_{n+1}(r, k) - \beta_n(r, k)$. Then from (31) we find

$$\Delta_1(r) = -k^{-2} \int_0^r V(t) \{ \sin^2\,[k(t + \eta_0 + \beta_1)] - \sin^2\,[k(t + \eta_0)] \}\,dt. \quad \text{(A29)}$$

Applying the mean-value theorem to the integrand in (A29) yields

$$\Delta_1(r) = -k^{-1}\int_0^r V(t)\beta_1(t)\sin \times \{2k[t+\eta_0+\psi(t)\beta_1]\}\,dt, \quad 0<\psi(t)<1. \tag{A30}$$

We now substitute (A28) into (A30) and obtain

$$\Delta_1(r) = -\frac{k}{3}\int_0^r V(t)\sin\{2k[t+\eta_0+\psi(t)\beta_1]\} \times \int_0^t V(\xi)(\xi+\eta_0)^4\cos[2k\theta(\xi)(\xi+\eta_0)]\,d\xi\,dt. \tag{A31}$$

Interchanging the order of integration in (A31) leads to

$$\Delta_1(r) = -\frac{k^2}{3}\int_0^r V(\xi)(\xi+\eta_0)^4\cos[2k\theta(\xi)(\xi+\eta_0)] \times \int_\xi^r V(t)k^{-1}\sin\{2k[t+\eta_0+\psi(t)\beta_1]\}\,dt\,d\xi. \tag{A32}$$

Finally we use the mean-value theorem again to write

$$\sin\{2k[t+\eta_0+\psi(t)\beta_1]\} = 2k[t+\eta_0+\psi(t)\beta_1] \times \cos\{2k\gamma(t)[t+\eta_0+\psi(t)\beta_1]\}, \quad 0<\gamma(t)<1. \tag{A33}$$

Upon using (A33) in (A32), and taking absolute values, we obtain

$$|\Delta_1(r)| \le \frac{2k^2}{3}\int_0^\infty |V(\xi)|\,|\xi+\eta_0|^4 \times \int_\xi^\infty |V(t)|\,(|t|+|\eta_0|+|\beta_1|)\,dt\,d\xi. \tag{A34}$$

Since $V(t) = O(t^{-4})$ and η_0 and β_1 are bounded as $t\to\infty$, the t integral in (A34) is $O(\xi^{-2})$ as $\xi\to\infty$. Therefore, the ξ integral converges, so (A34) shows that $\Delta_1(r) = O(k^2)$ uniformly in r.

Let us now make the inductive hypothesis that $\Delta_j(r) = O(k^2)$ and $\beta_j(r) = O(k)$ uniformly in r for $j = 1, 2, \cdots n$. We shall show that this implies $\Delta_{n+1}(r) = O(k^2)$ and $\beta_{n+1}(r) = O(k)$ uniformly in r. Since we have just proved that $\Delta_1(r) = O(k^2)$, the proof of (32) and (33) will be complete when we also show that $\beta_1(r) = O(k)$. We shall show this after considering the inductive step. We first observe that $\beta_{n+1} = \beta_n + \Delta_n$. From the inductive hypotheses it therefore follows that $\beta_{n+1}(r) = O(k)$. Thus we need merely consider Δ_{n+1}.

From (31) and the definition of Δ_{n+1} we have

$$\Delta_{n+1}(r) = -k^{-2}\int_0^r V(t)\{\sin^2[k(t+\eta_0+\beta_n)] - \sin^2[k(t+\eta_0+\beta_{n-1})]\}\,dt. \tag{A35}$$

Upon applying the mean-value theorem to the integrand, we obtain

$$\Delta_{n+1}(r) = -k^{-1}\int_0^r \Delta_n(t)V(t)\sin[2k(t+\eta_0)]\,dt - \int_0^r \beta_n^2(r)V(t)\cos\{2k[t+\eta_0+\delta_1(t)\beta_n]\}\,dt + \int_0^r \beta_{n-1}^2(r)V(t)\cos\{2k[t+\eta_0+\delta_2(t)\beta_{n-1}]\}\,dt, \quad 0<\delta_1(t),\,\delta_2(t)<1. \tag{A36}$$

Another application of the mean-value theorem to the sine function in the first integral, together with the fact that $\Delta_n(t) = O(k^2)$ uniformly in t, shows that this integral is $O(k^2)$. The other two integrals in (A36) are $O(k^2)$, since β_n and β_{n-1} are $O(k)$ uniformly in r. Thus $\Delta_{n+1}(r) = O(k^2)$ uniformly in r, which proves the inductive step.

To complete the induction we must show that $\beta_1(r) = O(k)$ uniformly in r. From the definition (31) of $\beta_1(r)$ we have

$$|\beta_1(r)| < k^{-2}\int_0^\infty |V(t)| \times |\sin^2(kt+k\eta_0) - (kt+k\eta_0)^2|\,dt. \tag{A37}$$

Rather than estimate the integral in (A37), we shall asymptotically evaluate $\beta_1(\infty)$, given by

$$\beta_1(\infty) = -k^{-2}\int_0^\infty V(t) \times \{\sin^2(kt+k\eta_0) - (kt+k\eta_0)^2\}\,dt. \tag{A38}$$

The method to be used on $\beta_1(\infty)$ also applies to (A37) and proves that $\beta_1 = O(k)$, but since we need the expansion of $\beta_1(\infty)$, the details for it are given.

We begin by introducing $\omega(k)$ as in Appendix II, with the properties that $\omega(k)\to\infty$ and $k\omega(k)\to 0$ as $k\to 0$. We also write $\beta_1(\infty) = I_1 + I_2$ where I_1 is k^{-2} times the integral in (A38) with upper limit ω, and I_2 involves the integral from ω to ∞.

To analyze I_1 we apply the mean-value theorem to the integrand to obtain

$$I_1 = \frac{k^2}{3}\int_0^\omega V(t)(t+\eta_0)^4\,dt - \frac{2}{45}k^4\int_0^\omega V(t)(t+\eta_0)^6 \times \cos[2\psi(t)(kt+k\eta_0)]\,dt, \quad 0<\psi(t)<1. \tag{A39}$$

As $\omega \to \infty$ both integrals in (A39) diverge. By using the fact that $V(t) \sim V_0 t^{-4}$ as $t \to \infty$ we can easily estimate the rate of divergence of these integrals to obtain

$$\int_0^\omega V(t)(t + \eta_0)^6 \cos [\psi(kt + k\eta_0)] = O(\omega^3) \quad \text{as} \quad \omega \to \infty, \tag{A40}$$

$$\int_0^\omega V(t)(t + \eta_0)^4 \sim V_0\omega + 4V_0\eta_0(\infty) \ln \omega + O(1) \quad \text{as} \quad \omega \to \infty. \tag{A41}$$

In obtaining (A41) we assumed that $V(t) = V_0 t^{-4} + O(t^{-6})$ as $t \to \infty$. From (A39) to (A41) we have

$$I_1 = \tfrac{1}{3}V_0k^2\omega + \tfrac{4}{3}V_0\eta_0(\infty)k^2 \ln \omega + O(k^2) + kO\{(k\omega)^3\}. \tag{A42}$$

In order to analyze I_2 we set $V(t) - V_0t^{-4} = \epsilon(t)$. Then

$$I_2 = -\frac{V_0}{k^2}\int_\omega^\infty t^{-4}\{\sin^2 [kt + k\eta_0] - k^2(t + \eta_0)^2\}\, dt - \frac{1}{k^2}\int_\omega^\infty \epsilon(t)\{\sin^2 [kt + k\eta_0] - k^2(t + \eta_0)^2\}\, dt. \tag{A43}$$

We estimate the second integral on the right in (A43) by first applying Taylor's expansion which yields

$$\sin^2 [kt + k\eta_0] - k^2(t + \eta_0)^2 = -k^4(t + \eta_0)^4 \cos [2\gamma(t)(kt + k\eta_0)], \quad 0 < \gamma < 1. \tag{A44}$$

Since $\epsilon(t) = O(t^{-6})$ as $t \to \infty$, it is clear that this second integral is $O(k^2)$.

The first integral in (A43) is analyzed by expanding the integrand in a Taylor expansion to write this term as a sum $I_2^{(1)} + I_2^{(2)} + I_2^{(3)}$, where

$$I_2^{(1)} = -\frac{V_0}{k^2}\int_\omega^\infty t^{-4}\{\sin^2 kt - k^2t^2\}\, dt, \tag{A45}$$

$$I_2^{(2)} = -\frac{V_0}{k}\int_\omega^\infty t^{-4}\eta_0(\sin 2kt - 2kt)\, dt, \tag{A46}$$

$$I_2^{(3)} = -V_0\int_\omega^\infty t^{-4}\eta_0^2\{\cos [2kt + 2\,\delta(t)k\eta_0] - 1\}\, dt, \quad 0 < \delta(t) < 1. \tag{A47}$$

We immediately note that

$$I_2^{(3)} = O(\omega^{-3}) \tag{A48}$$

To analyze $I_2^{(1)}$ we change the variable of integration to $y = kt$ and write $I_2^{(1)}$ as

$$I_2^{(1)} = -kV_0\int_0^\infty y^{-4}\{\sin^2 y - y^2\}\, dy + kV_0\int_0^{k\omega} y^{-4}\{\sin^2 y - y^2\}\, dy. \tag{A49}$$

The first integral in (A49) can be explicitly evaluated and has the value $-\pi/3$. The second integral can be expanded by Taylor's expansion to yield

$$I_2^{(1)} = kV_0\pi/3 - k^2V_0\omega/3 + kO[(k\omega)^3]. \tag{A50}$$

In order to analyze $I_2^{(2)}$ we first note from (9) that $\eta_0(t) \sim \eta_0(\infty) + O(t^{-1})$. By a now familiar application of Taylor's expansion to (A46), we can easily show that

$$I_2^{(2)} = -\frac{V_0\eta_0(\infty)}{k}\int_\omega^\infty t^{-4}(\sin 2kt - 2kt)\, dt + O(k^2) = -V_0\eta_0(\infty)k^2J + O(k^2). \tag{A51}$$

Here J is defined by

$$J = \int_{k\omega}^\infty y^{-4}(\sin 2y - 2y)\, dy. \tag{A52}$$

We now write

$$J = \int_{k\omega}^1 y^{-4}(\sin 2y - 2y)\, dy + \int_1^\infty y^{-4}(\sin 2y - 2y)\, dy. \tag{A53}$$

Upon applying Taylor's expansion to the first integral in (A53), we find

$$J = \tfrac{4}{3} \ln (k\omega) + O(1). \tag{A54}$$

Thus from (A51) and (A54) we have

$$I_2^{(2)} = -\tfrac{4}{3}V_0\eta_0(\infty)k^2 \ln (k\omega) + O(k^2). \tag{A55}$$

We now combine (A48), (A50), and (A55) to obtain

$$I_2 = kV_0\pi/3 - k^2V_0\omega/3 - \tfrac{4}{3}V_0\eta_0(\infty)k^2 \ln (k\omega) + O(\omega^{-3}) + kO[(k\omega)^3] + O(k^2), \tag{A56}$$

Upon recalling that $\beta_1(\infty) = I_1 + I_2$, we have from (A42) and (A56) that

$$\beta_1(\infty) = kV_0\pi/3 - \tfrac{4}{3}V_0\eta_0(\infty)k^2 \ln k + O(k^2) + O(\omega^{-3}) + kO[(k\omega)^3]. \tag{A57}$$

If we now choose $\omega = k^{-2/3}$, we see that the order terms in (A57) are all of order k^2. Thus (A57) is the desired result, which is given in the text by (34). In the application of the foregoing method to (A37) we note that the oscillatory character of the integrand played no role in determining the convergence properties of the integrals. The terms in I_1 and I_2

which canceled each other now no longer do so, but each term in I_1 and I_2 is $O(k)$ when $\omega = k^{-2/3}$, so therefore $\beta_1(r)$ is $O(k)$. This completes the asymptotic estimation of the iterates for the case $\nu = 4$.

Let us now consider $3\frac{1}{2} < \nu < 4$, for which (25) gives two terms in the expansion of $B(\infty, k)$. We shall now show that in this case $\beta(\infty, k) - B(\infty, k) = O(k^2)$. To do so we introduce the iterative solution for β just as in the case when $\nu = 4$. The integral in (A32) is convergent and $\Delta_1(r) = O(k^2)$ uniformly in r. The inductive hypothesis is made as before except that now we assume that $\beta_n(r) = O(k^{\nu-3})$ uniformly in r. We cannot use (A36) to conclude that $\Delta_{n+1}(r) = O(k^2)$. However, in order to make this conclusion we need only expand the integrand in (A35) to terms of order β_n^α and β_{n-1}^α where α is chosen so that $\alpha(\nu - 3) \geq 2$. The remainder term then will be of order k^2. The terms retained in the expansion will all have Δ_n as a factor and hence will be of order k^2.

Thus, in order to verify (25) we expand $\beta_1(\infty)$. Just as before the method will also apply to (A37) and show that $\beta_1 = O(k^{\nu-3})$. We proceed as in the case when $\nu = 4$ to define I_1 and I_2. To prevent needless rewriting we will indicate the changes in the analysis and then refer to the changed equations by denoting them with a prime. The order term in (A40) is to be replaced by $O(\omega^{7-\nu})$ and the right-hand side of (A41) is to be replaced by

$$\frac{V_0\omega^{5-\nu}}{5-\nu} + \frac{4\eta_0(\infty)}{4-\nu}\omega^{4-\nu} + O(1).$$

Consequently, from (A39), (A40′), and (A41′) we obtain

$$I_1 = \frac{V_0k^2\omega^{5-\nu}}{3(5-\nu)} + \frac{4V_0\eta_0(\infty)}{3(4-\nu)}k^2\omega^{4-\nu} + O(k^2) + O(k^4\omega^{7-\nu}) \qquad (A42')$$

In order to analyze I_2 we set $V(t) - V_0t^{-\nu} = \epsilon(t)$. Equation (A43) then is to be modified by replacing t^{-4} by $t^{-\nu}$. The integral in (A43) involving $\epsilon(t)$ is $O(k^2)$ as before. Equations (A45), (A46), and (A47) are to be modified by replacing t^{-4} by $t^{-\nu}$. The order term in (A48) is to be replaced by $O(\omega^{-\nu+1})$. Equation (A49) becomes

$$I_2^{(1)} = -k^{\nu-3}V_0\int_0^\infty y^{-\nu}\{\sin^2 y - y^2\}\,dy + k^{\nu-3}V_0\int_0^{k\omega} y^{-\nu}\{\sin^2 y - y^2\}\,dy, \qquad (A49')$$

and (A49) becomes

$$I_2^{(1)} = -k^{\nu-3}V_0\int_0^\infty y^{-\nu}\{\sin^2 y - y^2\}\,dy - \frac{V_0k^2\omega^{5-\nu}}{3(5-\nu)} + kO[(k\omega)^{7-\nu}]. \qquad (A50')$$

The analysis of $I_2^{(2)}$ proceeds exactly as before. We have

$$I_2^{(2)} = -\frac{V_0\eta_0(\infty)}{k}\int_\omega^\infty t^{-\nu}(\sin 2kt - 2kt)\,dt + O(k^2) = -V_0\eta_0(\infty)k^{\nu-2}J + O(k^2). \qquad (A51')$$

Here

$$J = \int_{k\omega}^\infty y^{-\nu}(\sin 2y - 2y)\,dy = \int_0^\infty y^{-\nu}(\sin 2y - 2y)\,dy - \frac{4}{3}\frac{(k\omega)^{4-\nu}}{(4-\nu)} + O[(k\omega)^{6-\nu}]. \qquad (A54')$$

Upon combining (A51′) and (A54′) we find

$$I_2^{(2)} = -k^{\nu-2}V_0\eta_0(\infty)\int_0^\infty y^{-\nu}(\sin 2y - 2y)\,dy + \frac{4}{3}\frac{V_0\eta_0(\infty)}{(4-\nu)}k^2\omega^{4-\nu} + O(k^2) + k^{\nu-2}O[(k\omega)^{6-\nu}]. \qquad (A55')$$

We now combine (A48′), (A50′), and (A55′) to obtain

$$I_2 = -k^{\nu-3}V_0\int_0^\infty y^{-\nu}\{\sin^2 y - y^2\}\,dy - k^{\nu-2}V_0\eta_0(\infty)\int_0^\infty y^{-\nu}(\sin 2y - 2y)\,dy - \frac{V_0k^2\omega^{5-\nu}}{3(5-\nu)} + \frac{4}{3}\frac{V_0\eta_0(\infty)}{(4-\nu)}k^2\omega^{4-\nu} + O(k^2) + k^{\nu-2}O[(k\omega)^{6-\nu}] + kO[(k\omega)^{7-\nu}] + O(\omega^{-\nu+1}) \qquad (A56')$$

Upon choosing $\omega = k^{-\alpha}$ with

$$\frac{\nu-2}{\nu-1} < \alpha < \frac{6-\nu}{7-\nu}$$

and combining (A42′) and (A56′), we find

$$\beta_1(\infty) = -k^{\nu-3}V_0\int_0^\infty y^{-\nu}\{\sin^2 y - y^2\}\,dy - k^{\nu-2}V_0\eta_0(\infty)\int_0^\infty y^{-\nu}(\sin 2y - 2y)\,dy + O(k^{\nu-2}). \qquad (A57')$$

Thus (A57′) is the desired result which is given in the text as (25).

The Diffraction of Waves By a Penetrable Ribbon*

C. YEH
Electrical Engineering Department, University of Southern California, Los Angeles, California
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The exact solution of the diffraction of waves by a dielectric ribbon or by an elliptical dielectric cylinder is obtained. Results are given in terms of Mathieu and modified Mathieu functions. It is found that each expansion coefficient of the scattered or transmitted wave is coupled to all coefficients of the series expansion for the incident wave, except when the elliptical cylinder degenerates to a circular one. Both polarizations of the incident wave are considered: one with the incident electric vector in the axial direction and the other with the incident magnetic vector in the axial direction. It is noted that the technique used in this paper to satisfy the boundary conditions may be applied to similar types of problems; such as the plasma-coated ribbon radiator and the corresponding acoustical problems.

I. INTRODUCTION

THE problems of scattering of waves by a circular cylinder have been considered by many authors.[1-3] The exact solution of the problem of the diffraction of waves by a perfectly conducting elliptical cylinder, or by a ribbon, has been obtained by Sieger,[4] and Morse and Rubenstein.[5] However, the corresponding solution for the diffraction of waves by a dielectric elliptical cylinder or by a dielectric ribbon has not been found. It is the purpose of this paper to present the exact solution of this problem. It is shown that certain mathematical difficulties can be overcome by separating the wave equation in elliptic cylinder coordinates and by applying the orthogonality properties of the Mathieu functions.

II. FORMULATION OF THE PROBLEM

To analyze this problem, the elliptical cylinder coordinated (ξ, η, z), as shown in Fig. 1, are introduced. In terms of the rectangular coordinates (x, y, z), the elliptical cylinder coordinates are defined by the following relations:

$$x = q \cosh \xi \cos \eta,$$
$$y = q \sinh \xi \sin \eta, \qquad (1)$$
$$z = z,$$
$$(0 \leq \xi < \infty, 0 \leq \eta \leq 2\pi),$$

where q is the semi-focal length of the ellipse. The contour surfaces of constant ξ are confocal elliptic cylinders, and those of constant η are confocal hyperbolic cylinders. One of the confocal elliptic cylinders with $\xi = \xi_0$ is assumed to coincide with the boundary of the solid dielectric cylinder, and z axis concides with its longitudinal axis. We shall consider waves whose propagation vector is in the x-y plane, so that the z coordinate may be omitted from the discussion. A possible solution of the wave equation is then $R(\xi)\Theta(\eta)e^{-i\omega t}$, where R and Θ satisfy the differential equations

$$d^2R/d\xi^2 - (c - 2\gamma^2 \cosh 2\xi)R = 0 \qquad (2)$$

$$d^2\Theta/d\eta^2 + (c - 2\gamma^2 \cos 2\eta)\Theta = 0, \qquad (3)$$

where c is the separation constant and $\gamma^2 = k^2q^2/4$, k being the wave number. Equations (2) and (3) are, respectively, the modified Mathieu and Mathieu differential equations.

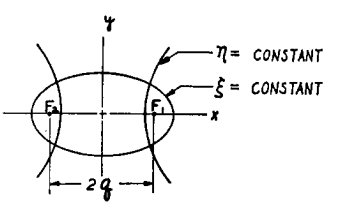

FIG. 1. The Elliptical cylinder coordinates. F_1 and F_2 are the foci of the ellipse. The distance between foci is the focal distance $2q$.

The periodic solutions of the equation in η are of two types: even about $\eta = 0$, and odd about $\eta = 0$. They are possible only for certain characteristic values of c. The even and odd functions are, respectively, denoted by $ce_n(\eta, \gamma^2)$ and $se_n(\eta, \gamma^2)$, with the sequence in n according to increasing values of c. It is noted that these functions are orthogonal functions. The solutions of (2) corresponding to the even function $ce_n(\eta, \gamma^2)$ having the same characteristic values of c are $Ce_n(\xi, \gamma^2)$ and $Fey_n(\xi, \gamma^2)$,

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and those corresponding to the odd function $se_n(\eta, \gamma^2)$ are $Se_n(\xi, \gamma^2)$ and $Gey_n(\xi, \gamma^2)$.[6]

The proper choice of these functions to represent the electromagnetic fields depends upon the boundary conditions. For the region within the dielectric cylinder, all field components must be finite. All field components for the scattered wave must satisfy the Sommerfeld's radiation condition at infinity. Consequently, the appropriate solutions of the wave equation for the region inside the dielectric cylinder are

$$\begin{Bmatrix} Ce_n(\xi, \gamma_1^2) & ce_n(\eta, \gamma_1^2) \\ Se_n(\xi, \gamma_1^2) & se_n(\eta, \gamma_1^2) \end{Bmatrix}, \tag{4}$$

and those for the scattered wave are

$$\begin{Bmatrix} Me_n^{(1),(2)}(\xi, \gamma_0^2) & ce_n(\eta, \gamma_0^2) \\ Ne_n^{(1),(2)}(\xi, \gamma_0^2) & se_n(\eta, \gamma_0^2) \end{Bmatrix}, \tag{5}$$

where

$$Me_n^{(1),(2)}(\xi, \gamma_0^2) = Ce_n(\xi, \gamma_0^2) \pm iFey_n(\xi, \gamma_0^2) \tag{6}$$

$$Ne_n^{(1),(2)}(\xi, \gamma_0^2) = Se_n(\xi, \gamma_0^2) \pm iGey_n(\xi, \gamma_0^2), \tag{7}$$

with

$$\gamma_0^2 = k_0^2 q^2/4 \quad \text{and} \quad \gamma_1^2 = k_1^2 q^2/4.$$
$$k_0^2 = \omega^2 \mu \epsilon_0 \quad \text{and} \quad k_1^2 = \omega^2 \mu \epsilon_1,$$

where ϵ_0 and ϵ_1 are, respectively, the dielectric constant of the free-space and of the elliptical cylinder.

III. SCATTERING OF A NORMALLY INCIDENT PLANE WAVE

Two types of normally incident waves are possible. One, called an E wave, is defined by $H_z = 0$, and the other, called an H wave, is defined by $E_z = 0$.

To simplify the notations for the Mathieu and modified Mathieu functions without any ambiguities, the following abbreviations are used:

$$\begin{aligned} ce_n(\eta) &= ce_n(\eta, \gamma_0^2), & se_n(\eta) &= se_n(\eta, \gamma_0^2), \\ ce_n^*(\eta) &= ce_n(\eta, \gamma_1^2), & se_n^*(\eta) &= se_n(\eta, \gamma_1^2), \\ Ce_n(\xi) &= Ce_n(\xi, \gamma_0^2), & Se_n(\xi) &= Se_n(\xi, \gamma_0^2), \\ Ce_n^*(\xi) &= Ce_n(\xi, \gamma_1^2), & Se_n^*(\xi) &= Se_n(\xi, \gamma_1^2), \\ Me_n^{(1),(2)}(\xi) &= Me_n^{(1),(2)}(\xi, \gamma_0^2), \\ Ne_n^{(1),(2)}(\xi) &= Ne_n^{(1),(2)}(\xi, \gamma_0^2). \end{aligned} \tag{8}$$

[6] We follow the notations adopted by Ince, [N. McLachlan, *Theory and Application of Mathieu Functions* (Oxford University Press, New York, 1951)].

It can be shown that the incident field of a plane wave with propagation vector in the x-y plane and at an angle θ with the x axis is proportional to the factor

$$e^{ik_0(x\cos\theta + y\sin\theta)} = e^{ik_0 q(\cosh\xi\cos\eta\cos\theta + \sinh\xi\sin\eta\sin\theta)}$$
$$= 2\sum_{n=0}^{\infty}\Big[\frac{1}{p_{2n}} Ce_{2n}(\xi)ce_{2n}(\eta)ce_{2n}(\theta)$$
$$+ (1/s_{2n+2})Se_{2n+2}(\xi)se_{2n+2}(\eta)se_{2n+2}(\theta)$$
$$+ (i/p_{2n+1})Ce_{2n+1}(\xi)ce_{2n+1}(\eta)ce_{2n+1}(\theta)$$
$$+ (i/s_{2n+1})Se_{2n+1}(\xi)se_{2n+1}(\eta)se_{2n+1}(\theta)\Big]. \tag{9}$$

where p_{2n}, p_{2n+1}, s_{2n+1}, and s_{2n+2} are joining factors.[6]

E wave. For an E wave, the field components of an incident wave are:

$$E_z^i = E_0\,\{\text{the right-hand side of Eq. (9)}\}, \tag{10}$$

$$H_\eta^i = (1/k_0^2 p)\{-i\omega\epsilon_0\,\partial E_z^i/\partial\xi\}. \tag{11}$$

$$H_\xi^i = (1/k_0^2 p)\{-i\omega\epsilon_0\,\partial E_z^i/\partial\eta\}, \tag{12}$$

where $p = q\,(\sinh^2\xi + \sin^2\eta)^{1/2}$. Referring to (4) and (5), we see that the scattered field and the transmitted field inside the dielectric cylinder must be of the form

$$E_z^s = 2E_0\sum_{n=0}^{\infty}\Big[\frac{A_{2n}}{p_{2n}} Me_{2n}^{(1)}(\xi)ce_{2n}(\eta)ce_{2n}(\theta)$$
$$+ (B_{2n+2}/s_{2n+2})Ne_{2n+2}^{(1)}(\xi)se_{2n+2}(\eta)se_{2n+2}(\theta)$$
$$+ i(A_{2n+1}/p_{2n+1})Me_{2n+1}^{(1)}(\xi)ce_{2n+1}(\eta)ce_{2n+1}(\theta)$$
$$+ i(B_{2n+1}/s_{2n+1})Ne_{2n+1}^{(1)}(\xi)se_{2n+1}(\eta)se_{2n+1}(\theta)\Big], \tag{13}$$

$$H_\eta^s = (1/k_0^2 p)\{-i\omega\epsilon_0\,\partial E_z^s/\partial\xi\}, \tag{14}$$

$$H_\xi^s = (1/k_0^2 p)\{-i\omega\epsilon_0\,\partial E_z^s/\partial\eta\}, \tag{15}$$

and

$$E_z^t = 2E_0\sum_{n=0}^{\infty}\Big[\frac{C_{2n}}{p_{2n}^*} Ce_{2n}^*(\xi)ce_{2n}^*(\eta)ce_{2n}(\theta)$$
$$+ (D_{2n+2}/s_{2n+2}^*)Se_{2n+2}^*(\xi)se_{2n+2}^*(\eta)se_{2n+2}(\theta)$$
$$+ i(C_{2n+1}/p_{2n+1}^*)Ce_{2n+1}^*(\xi)ce_{2n+1}^*(\eta)ce_{2n+1}(\theta)$$
$$+ i(D_{2n+1}/s_{2n+1}^*)Se_{2n+1}^*(\xi)se_{2n+1}^*(\eta)se_{2n+1}(\theta)\Big], \tag{16}$$

$$H_\eta^t = (1/k_1^2 p)\{-i\omega\epsilon_1\,\partial E_z^t/\partial\xi\}, \tag{17}$$

$$H_\xi^t = (1/k_1^2 p)\{-i\omega\epsilon_1\,\partial E_z^t/\partial\eta\}, \tag{18}$$

where A_{2n}, A_{2n+1}, B_{2n+2}, B_{2n+1}, C_{2n}, C_{2n+1}, D_{2n+2}, and D_{2n+1} are arbitrary unknown coefficients that can be determined by applying the boundary con-

ditions. p_{2n}^*, p_{2n+1}^*, s_{2n+2}^*, and s_{2n+1}^* are joining factors.[6]

The boundary conditions require the continuity of the tangential components of the electric and magnetic field at the boundary surface $\xi = \xi_0$; i.e.,

$$\begin{aligned}
&\sum_{n=0}^{\infty} [(g_{2n} + A_{2n}a_{2n})ce_{2n}(\eta) \\
&\quad + (h_{2n+2} + B_{2n+2}b_{2n+2})se_{2n+2}(\eta) \\
&\quad + i(g_{2n+1} + A_{2n+1}a_{2n+1})ce_{2n+1}(\eta) \\
&\quad + i(h_{2n+1} + B_{2n+1}b_{2n+1})se_{2n+1}(\eta)] \\
&= \sum_{n=0}^{\infty} \Bigg[C_{2n}c_{2n} \sum_{m=0}^{\infty} \alpha_{2n,2m}ce_{2m}(\eta) \\
&\quad + D_{2n+2}\, d_{2n+2} \sum_{m=0}^{\infty} \beta_{2n+2,2m+2}se_{2m+2}(\eta) \\
&\quad + iC_{2n+1}c_{2n+1} \sum_{m=0}^{\infty} \alpha_{2n+1,2m+1}ce_{2m+1}(\eta) \\
&\quad + i\, D_{2n+1}\, d_{2n+1} \sum_{m=0}^{\infty} \beta_{2n+1,2m+1}se_{2m+1}(\eta) \Bigg], \qquad (19)
\end{aligned}$$

$$\begin{aligned}
&\sum_{n=0}^{\infty} [(g'_{2n} + A_{2n}a'_{2n})ce_{2n}(\eta) \\
&\quad + (h'_{2n+2} + B_{2n+2}b'_{2n+2})se_{2n+2}(\eta) \\
&\quad + i(g'_{2n+1} + A_{2n+1}a'_{2n+1})ce_{2n+1}(\eta) \\
&\quad + i(h'_{2n+1} + B_{2n+1}b'_{2n+1})se_{2n+1}(\eta)] \\
&= \sum_{n=0}^{\infty} \Bigg[C_{2n}c'_{2n} \sum_{m=0}^{\infty} \alpha_{2n,2m}ce_{2m}(\eta) \\
&\quad + D_{2n+2}\, d'_{2n+2} \sum_{m=0}^{\infty} \beta_{2n+2,2m+2}se_{2m+2}(\eta) \\
&\quad + iC_{2n+1}c'_{2n+1} \sum_{m=0}^{\infty} \alpha_{2n+1,2m+1}ce_{2m+1}(\eta) \\
&\quad + i\, D_{2n+1}\, d'_{2n+1} \sum_{m=0}^{\infty} \beta_{2n+1,2m+1}se_{2m+1}(\eta) \Bigg], \qquad (20)
\end{aligned}$$

in which the relations

$$\begin{aligned}
ce_{2n}^*(\eta) &= \sum_{m=0}^{\infty} \alpha_{2n,2m}ce_{2m}(\eta), \\
se_{2n+2}^*(\eta) &= \sum_{m=0}^{\infty} \beta_{2n+2,2m+2}se_{2m+2}(\eta), \\
ce_{2n+1}^*(\eta) &= \sum_{m=0}^{\infty} \alpha_{2n+1,2m+1}ce_{2m+1}(\eta), \\
se_{2n+1}^*(\eta) &= \sum_{m=0}^{\infty} \beta_{2n+1,2m+1}se_{2m+1}(\eta),
\end{aligned} \qquad (21)$$

and the abbreviations

$$\begin{aligned}
h_l &= (1/s_l)Se_l(\xi_0)se_l(\theta), \\
h'_l &= (1/s_l)Se'_l(\xi_0)se_l(\theta), \\
g_l &= (1/p_l)Ce_l(\xi_0)ce_l(\theta), \\
g'_l &= (1/p_l)Ce'_l(\xi_0)ce_l(\theta), \\
a_l &= (1/p_l)Me_l^{(1)}(\xi_0)ce_l(\theta), \\
a'_l &= (1/p_l)Me_l^{(1)\prime}(\xi_0)ce_l(\theta), \\
b_l &= (1/s_l)Ne_l^{(1)}(\xi_0)se_l(\theta), \\
b'_l &= (1/s_l)Ne_l^{(1)\prime}(\xi_0)se_l(\theta), \\
c_l &= (1/p_l^*)Ce_l^*(\xi_0)ce_l(\theta), \\
c'_l &= (1/p_l^*)Ce_l^{*\prime}(\xi_0)ce_l(\theta), \\
d_l &= (1/s_l^*)Se_l^*(\xi_0)se_l(\theta), \\
d'_l &= (1/s_l^*)Se_l^{*\prime}(\xi_0)se_l(\theta), \\
&(l = 0, 1, 2, \cdots)
\end{aligned} \qquad (22)$$

have been used. The primes denote differentiation with respect to ξ_0. $\alpha_{2n,2m}$, $\alpha_{2n+1,2m+1}$, $\beta_{2n+2,2m+2}$, and $\beta_{2n+1,2m+1}$ are given in the Appendix. Applying the orthogonality relations of the Mathieu functions to Eq. (19) gives the following expressions:

$$g_{2j} + A_{2j}a_{2j} = \sum_{r=0}^{\infty} c_{2r}\alpha_{2r,2j}C_{2r} \qquad (23a)$$

$$g_{2j+1} + A_{2j+1}a_{2j+1} = \sum_{r=0}^{\infty} c_{2r+1}\alpha_{2r+1,2j+1}C_{2r+1} \qquad (23b)$$

$$h_{2j+2} + B_{2j+2}b_{2j+2} = \sum_{r=0}^{\infty} d_{2r+2}\beta_{2r+2,2j+2}\, D_{2r+2} \qquad (23c)$$

$$h_{2j+1} + B_{2j+1}b_{2j+1} = \sum_{r=0}^{\infty} d_{2r+1}\beta_{2r+1,2j+1}\, D_{2r+1} \qquad (23d)$$

$$(j = 0, 1, 2 \cdots).$$

Similarly; from Eq. (20) one contains the following expressions:

$$g'_{2j} + A_{2j}a'_{2j} = \sum_{r=0}^{\infty} c'_{2r}\alpha_{2r,2j}C_{2r}, \qquad (24a)$$

$$g'_{2j+1} + A_{2j+1}a'_{2j+1} = \sum_{r=0}^{\infty} c'_{2r+1}\alpha_{2r+1,2j+1}C_{2r+1} \qquad (24b)$$

$$h'_{2j+2} + B_{2j+2}b'_{2j+2} = \sum_{r=0}^{\infty} d'_{2r+2}\beta_{2r+2,2j+2}\, D_{2r+2}, \qquad (24c)$$

$$h'_{2j+1} + B_{2j+1}b'_{2j+1} = \sum_{r=0}^{\infty} d'_{2r+1}\beta_{2r+1,2j+1}\, D_{2r+1} \qquad (24d)$$

$$(j = 0, 1, 2 \cdots).$$

Solving these equations for the arbitrary constants C_{2r}, C_{2r+1}, D_{2r+1} and D_{2r+2}, one obtains in matrix notations,

$$C_{2r} = R^{-1}_{2r,2j}G_{2j}, \qquad (25a)$$

$$C_{2r+1} = R^{-1}_{2r+1,2j+1} G_{2j+1}, \tag{25b}$$

$$D_{2r+1} = Q^{-1}_{2r+1,2j+1} H_{2j+1}, \tag{25c}$$

$$D_{2r+2} = Q^{-1}_{2r+2,2j+2} H_{2j+2}, \tag{25d}$$

where $R^{-1}_{2r,2j}$ is the inverse of the matrix

$$R_{2j,2r} = (c_{2r} - c'_{2r} a_{2j}/a'_{2j})\alpha_{2r,2j};$$

$R^{-1}_{2r+1,2j+1}$ is the inverse of the matrix

$$R_{2j+1,2r+1} = (c_{2r+1} - c'_{2r+1} a_{2j+1}/a'_{2j+1})\alpha_{2r+1,2j+1};$$

$Q^{-1}_{2r+1,2j+1}$ is the inverse of the matrix

$$Q_{2j+1,2r+1} = (d_{2r+1} - d'_{2r+1} b_{2j+1}/b'_{2j+1})\beta_{2r+1,2j+1};$$

$Q^{-1}_{2r+2,2j+2}$ is the inverse of the matrix

$$Q_{2j+2,2r+2} = (d_{2r+2} - d'_{2r+2} b_{2j+2}/b'_{2j+2})\beta_{2r+2,2j+2};$$

$G_{2j} = g_{2j} - g'_{2j}\, a_{2j}/a'_{2j}$ is a column matrix; $G_{2j+1} = g_{2j+1} - g'_{2j+1}\, a_{2j+1}/a'_{2j+1}$ is a column matrix; $H_{2j+1} = h_{2j+1} - h'_{2j+1}\, b_{2j+1}/b'_{2j+1}$ is a column matrix; and

$$H'_{2j+2} = h_{2j+2} - h'_{2j+2} b_{2j+2}/b'_{2j+2}$$

is a column matrix. The other arbitrary constants can be easily obtained from Eq. (23) or (24); they are

$$A_{2j} = \frac{1}{a_{2j}}\left[-g_{2j} + \sum_{r=0}^{\infty} c_{2r}\alpha_{2r,2j} C_{2r}\right], \tag{25e}$$

$$A_{2j+1} = \frac{1}{a_{2j+1}}\left[-g_{2j+1} + \sum_{r=0}^{\infty} c_{2r+1}\alpha_{2r+1,2j+1} C_{2r+1}\right], \tag{25f}$$

$$B_{2j+1} = \frac{1}{b_{2j+1}}\left[-h_{2j+1} + \sum_{r=0}^{\infty} d_{2r+1}\beta_{2r+1,2j+1}\, D_{2r+1}\right], \tag{25g}$$

$$B_{2j+2} = \frac{1}{b_{2j+2}}\left[-h_{2j+2} + \sum_{r=0}^{\infty} d_{2r+2}\beta_{2r+2,2j+2}\, D_{2r+2}\right]. \tag{25h}$$

H wave. The expressions for the field components of an incident H wave are:

$$H^i_z = H_0\,\{\text{the right-hand side of Eq. (9)}\}, \tag{26}$$

$$E^i_\eta = (1/k_0^2 p)\{-i\omega\mu\ \partial H^i_z/\partial\xi\}, \tag{27}$$

$$E^i_\xi = (1/k_0^2 p)\{i\omega\mu\ \partial H^i_z/\partial\eta\}. \tag{28}$$

The scattered field and the transmitted field inside the dielectric cylinder are of the form

$$H^s_z = 2H_0 \sum_{n=0}^{\infty}\left[\frac{U_{2n}}{p_{2n}} Me^{(1)}_{2n}(\xi)ce_{2n}(\eta)ce_{2n}(\theta) + (V_{2n+2}/s_{2n+2})Ne^{(1)}_{2n+2}(\xi)se_{2n+2}(\eta)se_{2n+2}(\theta) + i(U_{2n+1}/p_{2n+1})Me^{(1)}_{2n+1}(\xi)ce_{2n+1}(\eta)ce_{2n+1}(\theta) + i(V_{2n+1}/s_{2n+1})Ne^{(1)}_{2n+1}(\xi)se_{2n+1}(\eta)se_{2n+1}(\theta)\right], \tag{29}$$

$$E^s_\eta = (1/k_0^2 p)\{-i\omega\mu\ \partial H^s_z/\partial\xi\}, \tag{30}$$

$$E^s_\xi = (1/k_0^2 p)\{i\omega\mu\ \partial H^s_z/\partial\eta\}, \tag{31}$$

and,

$$H^t_z = 2H_0 \sum_{n=0}^{\infty}\left[\frac{W_{2n}}{p^*_{2n}} Ce^*_{2n}(\xi)ce^*_{2n}(\eta)ce_{2n}(\theta) + (X_{2n+2}/s^*_{2n+2})Se^*_{2n+2}(\xi)se^*_{2n+2}(\eta)se_{2n+2}(\theta) + i(W_{2n+1}/p^*_{2n+1})Ce^*_{2n+1}(\xi)ce^*_{2n+1}(\eta)ce_{2n+1}(\theta) + i(X_{2n+1}/s^*_{2n+1})Se^*_{2n+1}(\xi)se^*_{2n+1}(\eta)se_{2n+1}(\theta)\right]. \tag{32}$$

$$E^t_\eta = (1/k_1^2 p)\{-i\omega\mu\ \partial H^t_z/\partial\xi\}, \tag{33}$$

$$E^t_\xi = (1/k_1^2 p)\{i\omega\mu\ \partial H^t_z/\partial\eta\}. \tag{34}$$

The unknown coefficients U_{2n}, U_{2n+1}, V_{2n+2}, V_{2n+1}, W_{2n}, W_{2n+1}, X_{2n+2}, and X_{2n+1} are to be determined by applying the boundary conditions that the tangential components of the magnetic and electric fields are continuous at the boundary surface $\xi = \xi_0$. Applying the similar procedures as described for the E wave, one obtains the following expressions for the arbitrary constants (in matrix notations):

$$W_{2r} = P^{-1}_{2r,2j} L_{2j}, \tag{35a}$$

$$W_{2r+1} = P^{-1}_{2r+1,2j+1} L_{2j+1}, \tag{35b}$$

$$X_{2r+1} = S^{-1}_{2r+1,2j+1} M_{2j+1}, \tag{35c}$$

$$X_{2r+2} = S^{-1}_{2r+2,2j+2} M_{2j+2}, \tag{35d}$$

$$U_{2j} = \frac{1}{a_{2j}}\left[-g_{2j} + \sum_{r=0}^{\infty} c_{2r}\alpha_{2r,2j} W_{2r}\right], \tag{35e}$$

$$U_{2j+1} = \frac{1}{a_{2j+1}}\left[-g_{2j+1} + \sum_{r=0}^{\infty} c_{2r+1}\alpha_{2r+1,2j+1} W_{2r+1}\right], \tag{35f}$$

$$V_{2j+1} = \frac{1}{b_{2j+1}}\left[-h_{2j+1} + \sum_{r=0}^{\infty} d_{2r+1}\beta_{2r+1,2j+1} X_{2r+1}\right], \tag{35g}$$

$$V_{2j+2} = \frac{1}{b_{2j+2}}\left[-h_{2j+2} + \sum_{r=0}^{\infty} d_{2r+2}\beta_{2r+2,2j+2} X_{2r+2}\right], \tag{35h}$$

where $P^{-1}_{2r,2j}$ is the inverse of the matrix

$$P_{2j,2r} = \left(c_{2r} - c'_{2r}\frac{a_{2j}}{a'_{2j}}\frac{\epsilon_0}{\epsilon_1}\right)\alpha_{2r,2j};$$

$P^{-1}_{2r+1,2j+1}$ is the inverse of the matrix

$$P_{2j+1,2r+1} = \left(c_{2r+1} - c'_{2r+1}\frac{a_{2j+1}}{a'_{2j+1}}\frac{\epsilon_0}{\epsilon_1}\right)\alpha_{2r+1,2j+1};$$

$S^{-1}_{2r+1,2j+1}$ is the inverse of the matrix

$$S_{2j+1,2r+1} = \left(d_{2r+1} - d'_{2r+1}\frac{b_{2j+1}}{b'_{2j+1}}\frac{\epsilon_0}{\epsilon_1}\right)\beta_{2r+1,2j+1};$$

$S^{-1}_{2r+2,2j+2}$ is the inverse of the matrix

$$S_{2j+2,2r+2} = \left(d_{2r+2} - d'_{2r+2}\frac{b_{2r+2}}{b'_{2r+2}}\frac{\epsilon_0}{\epsilon_1}\right)\beta_{2r+2,2j+2};$$

$L_{2j} = g_{2j} - g'_{2j}\,a_{2j}/a'_{2j}$ is a column matrix; $L_{2j+1} = g_{2j+1} - g'_{2j+1}\,a_{2j+1}/a'_{2j+1}$ is a column matrix; $M_{2j+1} = h_{2j+1} - h'_{2j+1}\,b_{2j+1}/b'_{2j+1}$ is a column matrix; and $M_{2j+2} = h_{2j+2} - h'_{2j+2}\,b_{2j+2}/b'_{2j+2}$ is a column matrix.

At large distance from the dielectric cylinder, the confocal ellipses are now sensibly concentric circles, and it is permissible to use the following asymptotic expressions for the radial Mathieu functions when $k_0r \gg 1$ and $k_0r \gg M$, where M is the order of the Mathieu function and $\frac{1}{4}k_0^2q^2\cosh^2\xi \approx \frac{1}{4}k_0^2r^2$:

$$Me^{(1)}_{2n}(\xi) \sim -ip_{2n}(2/\pi k_0r)^{1/2}e^{[i(k_0r+\pi/4)]}, \tag{36}$$

$$Me^{(1)}_{2n+1}(\xi) \sim -p_{2n+1}(2/\pi k_0r)^{1/2}e^{[i(k_0r+\pi/4)]}, \tag{37}$$

$$Ne^{(1)}_{2n+1}(\xi) \sim -s_{2n+1}(2/\pi k_0r)^{1/2}e^{[i(k_0r+\pi/4)]}, \tag{38}$$

$$Ne^{(1)}_{2n+2}(\xi) \sim -is_{2n+2}(2/\pi k_0r)^{1/2}e^{[i(k_0r+\pi/4)]}. \tag{39}$$

Using the above equations, one obtains the expressions for the far-zone scattered field:

$$H^s_\eta(E\text{ wave}) \approx 2E_0\left[(-i)\left(\frac{\epsilon_0}{\mu}\right)^{1/2}\right]\left(\frac{2}{\pi k_0r}\right)^{1/2}e^{i(k_0r+\pi/4)} \times \sum_{n=0}^{\infty}[A_{2n}ce_{2n}(\eta)ce_{2n}(\theta) + B_{2n+2}se_{2n+2}(\eta)se_{2n+2}(\theta) + A_{2n+1}ce_{2n+1}(\eta)ce_{2n+1}(\theta) + B_{2n+1}se_{2n+1}(\eta)se_{2n+1}(\theta)], \tag{40}$$

$$E^s_\eta(H\text{ wave}) \approx 2H_0\left[(-i)\left(\frac{\mu}{\epsilon_0}\right)^{1/2}\right]\left(\frac{2}{\pi k_0r}\right)^{1/2}e^{i(k_0r+\pi/4)} \times \sum_{n=0}^{\infty}[U_{2n}ce_{2n}(\eta)ce_{2n}(\theta) + V_{2n+2}se_{2n+2}(\eta)se_{2n+2}(\theta) + U_{2n+1}ce_{2n+1}(\eta)ce_{2n+1}(\theta) + V_{2n+1}se_{2n+1}(\eta)se_{2n+1}(\theta)]. \tag{41}$$

The ribbon corresponds to the limiting case of a cylinder of very small thickness, $\xi_0 \to 0$.

As an ellipse degenerates to a circle its semifocal length q tends to zero while ξ_0 approaches infinity such that the product $q\cosh\xi_0$ or $q\sinh\xi_0$ or $\frac{1}{2}qe^{\xi_0}$ tends to a constant r_0, which is the radius of the degenerated circle. Using the degenerated forms of Mathieu and modified Mathieu functions,[6] the arbitrary constants for the E wave become

$$C_s = D_s = \frac{H^{(1)\prime}_s(k_0r_0)J_s(k_0r_0) - J'_s(k_0r_0)H^{(1)}_s(k_0r_0)}{H^{(1)\prime}_s(k_0r_0)J_s(k_1r_0) - (\epsilon_1/\epsilon_0)^{1/2}J'_s(k_1r_0)H^{(1)}_s(k_0r_0)}, \tag{42a}$$

$$A_s = B_s = \frac{(\epsilon_1/\epsilon_0)^{1/2}J_s(k_0r_0)J'_s(k_1r_0) - J'_s(k_0r_0)J_s(k_1r_0)}{H^{(1)\prime}_s(k_0r_0)J_s(k_1r_0) - (\epsilon_1/\epsilon_0)^{1/2}J'_s(k_1r_0)H^{(1)}_s(k_0r_0)}, \tag{42b}$$

and the arbitrary constants for the H wave become

$$W_s = X_s = \frac{H^{(1)\prime}_s(k_0r_0)J_s(k_0r_0) - J'_s(k_0r_0)H^{(1)}_s(k_0r_0)}{H^{(1)\prime}_s(k_0r_0)J_s(k_1r_0) - J'_s(k_1r_0)H^{(1)}_s(k_0r_0)(\epsilon_0/\epsilon_1)^{1/2}}, \tag{43a}$$

$$U_s = V_s = \frac{(\epsilon_0/\epsilon_1)^{1/2}J_s(k_0r_0)J'_s(k_1r_0) - J'_s(k_0r_0)J_s(k_1r_0)}{H^{(1)\prime}_s(k_0r_0)J_s(k_1r_0) - J'_s(k_1r_0)H^{(1)}_s(k_0r_0)(\epsilon_0/\epsilon_1)^{1/2}}. \tag{43b}$$

These are well-known expressions for the circular dielectric cylinder. This completes the derivation of the fundamental formulae involved in the diffraction of waves by an elliptical dielectric cylinder.

IV. CONCLUSION

The exact solution of the problem of the diffraction of waves by an elliptical dielectric cylinder, or by a dielectric ribbon is obtained. It is interesting to note that unlike the case for a circular dielectric cylinder, or the case for a perfectly conducting elliptical cylinder, each expansion coefficient of the scattered or transmitted wave for the dielectric elliptical cylinder is coupled to all coefficients of the series expansion for the incident wave. This characteristic is also found in the problem of surface wave propagation along an elliptical dielectric cylinder.[7] To qualitatively illustrate how the solutions behave, the radiation patterns of the scattered fields for the two polarizations of the incident wave are

[7] C. Yeh, Ph.D. Thesis, California Institute of Technology, Pasadena, California, 1962; J. Appl. Phys. 33, 3235 (1962).

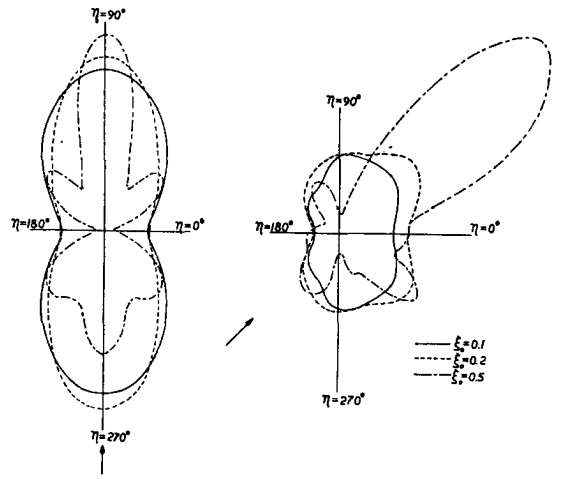

FIG. 2. Polar diagrams for waves ($|H_\eta^s|$) scattered by a dielectric ribbon with $k_0^2q^2 = 10$. The incident electric vector is polarized in the axial direction. (Arrows indicate the direction of incident waves.)

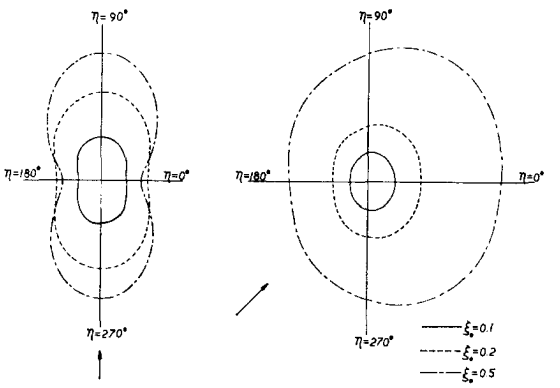

FIG. 3. Polar diagrams for waves ($|H_\eta^s|$) scattered by a dielectric ribbon with $k_0^2\ q^2 = 1.0$. The incident electric vector is polarized in the axial direction. (Arrows indicate the direction of incident waves.)

computed. Numerical computations are carried out using the available tables on the expansion coefficients of Mathieu functions,[8] and using the high-speed IBM 7090 computer. Two cases of k_0q are considered: one with $k_0q = 1$, and the other with $k_0q = (10)^{1/2}$. Various values of ξ_0 are used. It is assumed that $\epsilon_1/\epsilon_0 = 2.0$. Results are shown in Figs. 2 through 5. Numerical investigation shows that the infinite series representing these expansion coefficients for the scattered or transmitted wave converge quite rapidly for small values of $\gamma_1 = k_1q/2$; only the first few terms of the infinite series are needed as long as γ_1 is less than 4. The rate of convergence can best be illustrated by the example in Table I, where A_{2n}, A_{2n+1}, B_{2n+2}, and B_{2n+1} are

TABLE I. The rate of convergence for $\xi_0 = 0.2$, $k_0q = (10)^{1/2}$, and $\theta = 90°$.

	A_{2n}			A_{2n+1}		
n	$m = 5$	$m = 6$	$m = 7$	$m = 5$	$m = 6$	$m = 7$
0	-0.215×10	-0.218×10	-0.218×10	-0.477×10	-0.482×10	-0.482×10
	$-0.280 \times 10i$	$-0.286 \times 10i$	$-0.287 \times 10i$	$-0.479 \times 10i$	$-0.484 \times 10i$	$-0.485 \times 10i$
1	-0.346×10	-0.354×10	-0.355×10	-0.176×10	-0.178×10	-0.178×10
	$+0.583i$	$+0.594i$	$+0.595i$	$+0.551i$	$+0.556i$	$+0.557i$
2	-0.503	-0.516	-0.518	-0.142×10^{-1}	-0.143×10^{-1}	-0.143×10^{-1}
	$+0.693i$	$+0.711i$	$+0.713i$	$+0.896 \times 10^{-1}i$	$+0.903 \times 10^{-1}i$	$+0.905 \times 10^{-1}i$
3	-0.417×10^{-2}	-0.433×10^{-2}	-0.435×10^{-2}	-0.313×10^{-4}	-0.319×10^{-4}	-0.319×10^{-4}
	$+0.547 \times 10^{-1}i$	$+0.572 \times 10^{-1}i$	$-0.575 \times 10^{-1}i$	$+0.399 \times 10^{-2}i$	$+0.411 \times 10^{-2}i$	$+0.412 \times 10^{-2}i$
4	-0.109×10^{-4}	-0.122×10^{-4}	-0.124×10^{-4}	-0.723×10^{-7}	-0.761×10^{-7}	-0.766×10^{-7}
	$+0.260 \times 10^{-2}i$	$+0.303 \times 10^{-2}i$	$+0.310 \times 10^{-2}i$	$+0.160 \times 10^{-3}i$	$+0.179 \times 10^{-3}i$	$+0.181 \times 10^{-3}i$
5		-0.174×10^{-7}	-0.189×10^{-7}		-0.144×10^{-10}	-0.165×10^{-10}
		$+0.116 \times 10^{-3}i$	$+0.128 \times 10^{-3}i$		$+0.523 \times 10^{-5}i$	$+0.564 \times 10^{-5}i$
6			-0.168×10^{-10}			-0.216×10^{-13}
			$+0.377 \times 10^{-5}i$			$+0.129 \times 10^{-6}i$

	B_{2n+2}			B_{2n+1}		
n	$m = 5$	$m = 6$	$m = 7$	$m = 5$	$m = 6$	$m = 7$
0	-0.368×10^{-2}	-0.368×10^{-2}	-0.368×10^{-2}	-0.144×10^{-1}	-0.144×10^{-1}	-0.144×10^{-1}
	$+0.695 \times 10^{-1}i$	$+0.695 \times 10^{-1}i$	$+0.695 \times 10^{-1}i$	$+0.127i$	$+0.127i$	$+0.127i$
1	-0.736×10^{-4}	-0.736×10^{-4}	-0.736×10^{-4}	-0.179×10^{-2}	-0.180×10^{-2}	-0.180×10^{-2}
	$+0.859 \times 10^{-2}i$	$+0.859 \times 10^{-2}i$	$+0.859 \times 10^{-2}i$	$+0.445 \times 10^{-1}i$	$+0.446 \times 10^{-1}i$	$+0.446 \times 10^{-1}i$
2	-0.461×10^{-6}	-0.462×10^{-6}	-0.462×10^{-6}	-0.489×10^{-4}	-0.490×10^{-4}	-0.490×10^{-4}
	$+0.640 \times 10^{-3}i$	$+0.641 \times 10^{-3}i$	$+0.641 \times 10^{-3}i$	$+0.691 \times 10^{-2}i$	$+0.693 \times 10^{-2}i$	$+0.693 \times 10^{-2}i$
3	-0.105×10^{-8}	-0.106×10^{-8}	-0.106×10^{-8}	-0.279×10^{-6}	-0.282×10^{-6}	-0.282×10^{-6}
	$+0.301 \times 10^{-4}i$	$+0.304 \times 10^{-4}i$	$+0.304 \times 10^{-4}i$	$+0.499 \times 10^{-3}i$	$+0.500 \times 10^{-3}i$	$+0.501 \times 10^{-3}i$
4	-0.120×10^{-11}	-0.126×10^{-11}	-0.127×10^{-11}	-0.669×10^{-9}	-0.717×10^{-9}	-0.722×10^{-9}
	$+0.988 \times 10^{-6}i$	$+0.105 \times 10^{-5}i$	$+0.106 \times 10^{-5}i$	$+0.229 \times 10^{-4}i$	$+0.249 \times 10^{-4}i$	$+0.251 \times 10^{-4}i$
5		-0.763×10^{-15}	-0.797×10^{-15}		-0.693×10^{-12}	-0.731×10^{-12}
		$+0.255 \times 10^{-7}i$	$+0.268 \times 10^{-7}i$		$+0.763 \times 10^{-6}i$	$+0.811 \times 10^{-6}i$
6			-0.299×10^{-18}			-0.450×10^{-15}
			$+0.506 \times 10^{-9}i$			$+0.194 \times 10^{-7}i$

[8] National Bureau of Standards, *Tables Relating to Mathieu Functions* (Columbia University Press, New York, 1951).

the expansions coefficients for the scattered field H_η^s [see Eq. (40)]. $m \times m$ is the size of the matrix used. It is observed that the infinite series converge faster for smaller values of $k_0 q$ and ξ_0. For example, when $k_0 q = 1.0$, $\xi_0 = 0.2$, only three terms of the infinite series (i.e., $m = 3$) are required.

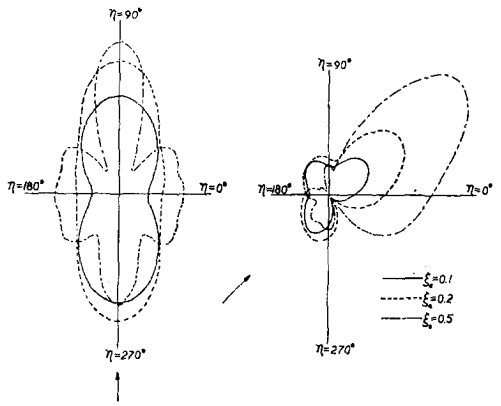

FIG. 4. Polar diagrams for waves ($|E_\eta^s|$) scattered by a dielectric ribbon with $k_0^2 q^2 = 10$. The incident magnetic vector is polarized in the axial direction. (Arrows indicate the direction of incident waves.)

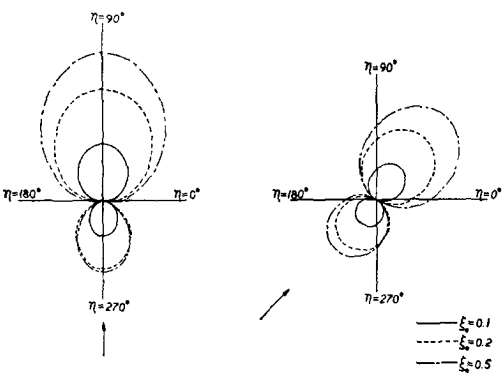

FIG. 5. Polar diagrams for waves ($|E_\eta^s|$) scattered by a dielectric ribbon with $k_0^2 q^2 = 1.0$. The incident magnetic vector is polarized in the axial direction. (Arrows indicate the direction of incident waves.)

It is interesting to note that the solutions with a slight modification are applicable to the problem of the diffraction of waves from a plasma ribbon, and that the method used in analyzing this problem are applicable to problems involving dielectric coated elliptical cylindrical radiators. Corresponding acoustical problems may also be analyzed in a similar manner.

ACKNOWLEDGMENTS

I would like to thank Miss Linda LaBella for typing this manuscript. I also wish to thank Mrs. G. Knudson and Mrs. K. K. Higa of the Hughes Aircraft Company in Culver City for providing the subroutines to compute Bessel functions and to invert matrix. The use of the computing facilities at the Western Data Processing Center at UCLA is gratefully acknowledged.

APPENDIX

FORMULAS FOR $\alpha_{2n,2m}$, $\alpha_{2n+1,2m+1}$, $\beta_{2n+2,2m+2}$, AND $\beta_{2n+1,2m+1}$

It can readily be shown, from the theory of Mathieu functions that

$$\alpha_{2n,2m} = \frac{\int_0^{2\pi} ce_{2n}^*(\eta) ce_{2m}(\eta)\, d\eta}{\int_0^{2\pi} ce_{2m}^2(\eta)\, d\eta} = \frac{2A_0^{*(2n)} A_0^{(2m)} + \sum_{r=1}^{\infty} [A_{2r}^{*(2n)} A_{2r}^{(2m)}]}{2[A_0^{(2m)}]^2 + \sum_{r=1}^{\infty} [A_{2r}^{(2m)}]^2},$$

$$\alpha_{2n+1,2m+1} = \frac{\int_0^{2\pi} ce_{2n+1}^*(\eta) ce_{2m+1}(\eta)\, d\eta}{\int_0^{2\pi} ce_{2m+1}^2(\eta)\, d\eta} = \frac{\sum_{r=0}^{\infty} [A_{2r+1}^{*(2n+1)} A_{2r+1}^{(2m+1)}]}{\sum_{r=0}^{\infty} [A_{2r+1}^{(2m+1)}]^2},$$

$$\beta_{2n+2,2m+2} = \frac{\int_0^{2\pi} se_{2n+2}^*(\eta) se_{2m+2}(\eta)\, d\eta}{\int_0^{2\pi} se_{2m+2}^2(\eta)\, d\eta} = \frac{\sum_{r=0}^{\infty} [B_{2r+2}^{*(2n+2)} B_{2r+2}^{(2m+2)}]}{\sum_{r=0}^{\infty} [B_{2r+2}^{(2m+2)}]^2},$$

$$\beta_{2n+1,2m+1} = \frac{\int_0^{2\pi} se_{2n+1}^*(\eta) se_{2m+1}(\eta)\, d\eta}{\int_0^{2\pi} se_{2m+1}^2(\eta)\, d\eta} = \frac{\sum_{r=0}^{\infty} [B_{2r+1}^{*(2n+1)} B_{2r+1}^{(2m+1)}]}{\sum_{r=0}^{\infty} [B_{2r+1}^{(2m+1)}]^2},$$

where

$A_{2r}^{(2n)}$, $A_{2r}^{*(2n)}$, $A_{2r+1}^{(2n+1)}$, $A_{2r+1}^{*(2n+1)}$, $B_{2r+2}^{(2n+2)}$, $B_{2r+2}^{*(2n+2)}$, $B_{2r+1}^{(2n+1)}$, and $B_{2r+1}^{*(2n+1)}$ are, respectively, the expansion coefficients for

$ce_{2n}(\eta)$, $ce_{2n}^*(\eta)$, $ce_{2n+1}(\eta)$, $ce_{2n+1}^*(\eta)$, $se_{2n+2}(\eta)$, $se_{2n+2}^*(\eta)$, $se_{2n+1}(\eta)$, and $se_{2n+1}^*(\eta)$ (see reference 6).

The Inverse Problem in the Quantum Theory of Scattering*

L. D. FADDEYEV

Translated from the Russian by

B. SECKLER

Pratt Institute, Brooklyn, New York

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This report is a translation from the Russian of a survey article by L. D. Faddeyev, which appeared in Uspekhi Matem. Nauk., **14**, 57 (1959). Our own interest in this article lies in its relevance to the inverse scattering problem—that is, the problem of determining information about a medium from which an electromagnetic wave is reflected, given a knowledge of the reflection coefficient. Similar questions concerning scattering phenomena in other branches of physics, e.g., in quantum mechanics, can be investigated by means of the same theory. We have therefore thought it worthwhile to reproduce and distribute the translation. A good indication of the contents is given in the Introduction.

INTRODUCTION

THIS paper is devoted to a survey of the following fundamental problem arising in the quantum theory of scattering: *The solution of*

$$L\psi = -(d^2/dx^2)\psi(x, k) + q(x)\psi(x, k) = k^2\psi(x, k), \tag{0.1}$$

satisfying the condition

$$\psi(0, k) = 0, \tag{0.2}$$

behaves asymptotically like

$$\psi(x, k) \approx C(k) \sin [kx - \eta(k)], \tag{0.3}$$

provided the potential $q(x)$ decreases sufficiently fast as x tends to infinity; to what extent does the assignment of $\eta(k)$ determine $q(x)$ and how are these functions related. This problem is one of the general questions concerning the relationship between the S matrix and the energy operator in scattering theory. The operator L, defined by Eq. (0.1) and condition (0.2), is the simplest example of the energy operator occurring in scattering theory, and the function $S(k) = e^{-2i\eta(k)}$ the simplest example of the S matrix or scattering operator.

First introduced by Wheeler, the S matrix has since been frequently used in scattering theory, particularly following the publication of Heisenberg's papers.[1] In these articles, the following time-independent definition of the S matrix was given. A wavefunction, describing the steady state of a system (for simplicity, we restrict ourselves to a system of two particles), has an asymptotic representation in the space variables

$$\Psi\,|_{r\to\infty} \approx \Psi_1 + \Psi_2, \tag{0.4}$$

where r is the distance between particles. Ψ_1 and Ψ_2 are, respectively, outgoing and incoming waves, so that Ψ_1 contains the factor e^{ikr} and Ψ_2 is proportional to e^{-ikr}, k being the wavenumber characterizing the energy of the state Ψ. The quantity relating the amplitudes of these two functions is called the S matrix. In our illustration,

$$\psi(x, k) \approx [C(k)/2i][e^{ikx-i\eta(k)} - e^{-ikx+i\eta(k)}], \tag{0.5}$$

i.e., the first term corresponds to an outgoing wave, the second to an incoming wave, and their amplitudes are related by the factor

$$S(k) = e^{-2i\eta(k)}, \tag{0.6}$$

the S matrix for our example.

Heisenberg's theory of the S matrix was further developed in two papers by Møller,[2] who gave a time-dependent definition of the S matrix that is physically more justified. Since then, this time-dependent formulation of the scattering problem has received a great deal of attention (see the Appendix) and can be stated in the following way: The energy operator of a system consists of two terms

$$L = L_0 + V, \tag{0.7}$$

where L_0 corresponds to the energy of the free particles and V to their interaction energy. Long before collision, i.e., for negatively infinite time, the state of the noninteracting particles is described by a vector $\Omega_-(t)$[3] whose dependence on time is determined by the operator L_0:

* The research in this paper was supported by the U. S. Air Force Cambridge Research Laboratories under Contract No. AF 19(604)3495.

[1] W. Heisenberg, Z. Physik **120**, 513–538, 673–702 (1943).

[2] C. Møller, Kgl. Danske Videnskab Selskab, Mat.-fys. Medd. **23**, No. 1 (1945), **22**, No. 19 (1946).

[3] In conformity with established terminology, a state *vector* will be understood to be an element of Hilbert space in which all operators act.

$$\Omega_-(t) = e^{-iL_0t}\Omega_-, \tag{0.8}$$

Ω_- being a constant vector characterizing the initial state of the system. For finite time, the state $\Omega(t)$ is a solution of the Schrödinger equation

$$i\,\partial\Omega(t)/\partial t = L\Omega(t) = (L_0 + V)\Omega(t), \tag{0.9}$$

and is required to take on the initial state $\Omega_-(t)$ in the sense

$$\lim_{t\to-\infty} ||\Omega(t) - \Omega_-(t)|| = 0. \tag{0.10}$$

Over a long interval of time after collision, the motion of the particles again becomes free, so that asymptotically,

$$||\Omega(t) - \Omega_+(t)|| \to 0, \qquad (t \to \infty), \tag{0.11}$$

where $\Omega_+(t) = e^{-iL_0t}\Omega_+$. The manner in which the asymptotic state vector changes, determines the nature of the scattering process. The operator S that relates the asymptotic vectors Ω_+ and Ω_- according to the formula

$$\Omega_+ = S\Omega_-, \tag{0.12}$$

is called the *scattering operator* or S matrix.

In Sec. 3, it will be shown that this formulation holds for the example in question, the S matrix being given by the function $S(k) = e^{-2i\eta(k)}$ occurring in the time-independent definition. This fact typifies a general aspect of the stationary and nonstationary formulations of the S matrix in case both definitions are valid.

Heisenberg came to consider the S matrix as a means of overcoming the difficulties encountered in modern relativistic theory of elementary particles. He felt it was necessary to introduce a new fundamental constant having dimension length. Therefore, he analyzed the current theory and rejected as unobservable those notions which contradict the idea of a fundamental length. Only those experimentally observable quantities would be put in a future theory. In this sense, the S matrix satisfies the requirements of Heisenberg. It describes the wave function at large distances and is thus not contrary to the hypothesis of a fundamental length. Moreover, the scattering cross section, which can be measured directly is expressible in terms of the elements of the S matrix. Heisenberg also conjectured that the discrete energy levels corresponding to bound states of the particles should be determined by the analytic continuation of the S matrix into the complex energy plane.

Connected with Heisenberg's supposition that the S matrix is more fundamental than the Hamiltonian is the question of clarifying the relationship between these two characterizations of a system. In particular, in what sense should one define the Hamiltonian on the basis of the S matrix when both of these notions are used in a theory. In addition to its theoretical aspect, the inverse problem, i.e., the reconstruction of the energy operator from its S matrix, could be of great practical value in the interpretation of experimental scattering data and in the determination of various properties of the particles which are not directly measurable.

The simplest example in scattering theory is the radial equation for the scattering by a fixed, spherically symmetric center:

$$-(d^2/dx^2)\psi(x, k) = [l(l+1)/x^2 + q(x)] \times \psi(x, k) = k^2\psi(x, k), \tag{0.13}$$

which, for $l = 0$, reduces to the case already mentioned. The first attempts at solving the inverse problem were undertaken by Frødberg[4] and Hylleraas.[5] They worked out a formal procedure using a series whose convergence is highly plausible. However, Bargmann[6] constructed explicit examples in which different potentials give rise to the same $S(k)$ and to the same discrete energy levels. This showed that a potential cannot be reconstructed uniquely from prescribed energy levels and scattering function $S(k)$. Levinson[7] showed that this lack of uniqueness is related to the existence of a discrete spectrum. To wit, he proved that the reconstructed potential is unique when there is no discrete spectrum. The precise mathematical reason for this was given by Marchenko[8] who showed that the S function[9] determines the continuous portion of the so-called spectral function of equation (0.1). To find the spectral function when there is a discrete spectrum, one must not only prescribe the location of the eigenvalues, but also the values of the derivatives of the corresponding normalized eigenfunctions, for example, at $x = 0$. Marchenko[10] also showed that the spectral function uniquely determines a potential. Thus, Marchenko related the problem in question to the inverse Sturm-Liouville problem which already had been treated in the mathematical

[4] C. E. Frødberg, Phys. Rev. **72**, 519 (1947).
[5] E. A. Hylleraas, Phys. Rev. **74**, 48 (1948).
[6] V. Bargmann, Phys. Rev. **75**, 301 (1949).
[7] N. Levinson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **25**, No. 9 (1949).
[8] V. A. Marchenko, Trudy Moskov. matem. o-va **1**, 327–420 (1952).
[9] We shall call the scattering operator in our example the S function.
[10] V. A. Marchenko, Doklady Akad. Nauk S. S. S. R. 72, 457 (1950).

literature. An analogous result was obtained at approximately the same time by Borg.[11] By developing Levinson's method, Jost and Kohn[12,13] independently came to the same conclusion concerning the reason for this lack of uniqueness. They gave an explicit formula for a family of potentials which [besides $q(x)$] yield the same S function and the same discrete energy levels. An analogous formula was obtained by Holmberg.[14]

A procedure for explicitly constructing a potential without the singularity $l(l+1)/x^2$ from its spectral function was formulated by Gel'fand and Levitan.[15] They reduced the problem to a linear integral equation and gave sufficient conditions in terms of the spectral function assuring that it be the spectral function of some equation with a potential from a given class. The results of Gel'fand and Levitan on the inverse Sturm-Liouville problem were immediately applied to the inverse scattering problem by Jost and Kohn[16] and by Levinson.[17] In reference 16, a formula was given for a family of equivalent potentials each having the same S function and discrete energy levels. More precise conditions (both necessary and sufficient) on the spectral function were obtained by Krein.[18] His paper completed the general problem of reconstructing Eq. (0.1) from its spectral function. However, since the passage from the S function to the spectral function is not entirely trivial, there still remained unanswered the question of characterizing the class of possible S functions corresponding to the potentials from a given class. This problem was solved by Krein[19] and Marchenko,[20] who showed that it is convenient to formulate conditions in terms of the Fourier transform of the function $S(k) - 1$. Marchenko showed that the potential $q(x)$ possesses the same properties for x tending to zero and infinity as does the derivative of this Fourier transform. Definitive inequalities obtained by Marchenko permitted him to formulate necessary and sufficient conditions on the S function, assuring that a potential from a given class would correspond to it.

After the basic papers of Gel'fand and Levitan, and Krein, and Marchenko, a great deal of work was devoted to extending their results to an equation containing the singular term $l(l+1)/x^2$, an equation over the interval $-\infty < x < \infty$, a system of equations, and the relativistic equations. A brief survey is given in the Appendix.

It is interesting to note that the inverse problem has been studied in the U.S.S.R. almost exclusively by mathematicians and elsewhere almost exclusively by physicists, who merely use the method of Gel'fand-Levitan as interpreted by Levinson, and by Jost and Kohn. An explanation of the general features of this method which permit its application to the solution of various problems, was undertaken in a series of papers by Kay and Moses.[21-24] These authors use the general concept of transformation operator developed by Friedrichs.[25,26]

Recently, work has been devoted to applying the results of the inverse problem in the interpretation of experimental scattering data.[27-29]

Thus, the inverse scattering problem for the simplest case of the radial equation has been solved in about a decade, and a large amount of literature is devoted to it. In this survey, we shall attempt to give the results of most of these papers and also in their most general form. This will make clearer the ways in which the basic results can be carried over to other problems. In this, an essential part will be played by the general approach to transformation operators developed by Friedrichs and applied to the inverse problem by Kay and Moses.

All of the basic results on the inverse scattering problem could be obtained by the use of one of the the methods of Gel'fand-Levitan, Marchenko, or Krein. Our presentation will not stick to any particular one of these approaches, but rather, at different points, will make use of different methods. We shall attempt to establish their connection considering that each of them explains different aspects of the mathematical structure of the whole problem.

Because of the large material content, not every

[11] G. Borg, "Uniqueness theorems in the spectral theory of $y'' + (\lambda - q(x))\, y = 0$," Eleventh Congress of Scandanavian Mathematics, held at Trondheim, August 22–25, 1949, pp. 276–287.
[12] R. Jost and W. Kohn, Phys. Rev. **87**, 979 (1952).
[13] R. Jost and W. Kohn, Phys. Rev. **88**, 382 (1952).
[14] B. Holmberg, Nuovo cimento **9**, 597 (1952).
[15] I. M. Gel'fand and B. M. Levitan, Izvest. Akad Nauk S. S. S. R. Ser. matem. **15**, 309–360 (1951).
[16] R. Jost and W. Kohn, Kgl Danske Videnskab. Selskab, Mat.-fys. Medd. **27**, No. 9 (1953).
[17] N. Levinson, Phys. Rev. **89**, 755–757 (1953).
[18] M. G. Krein, Doklady Akad. Nauk S. S. S. R. **88**, 405 (1953).
[19] M. G. Krein, Doklady Akad. Nauk S.S.S.R. **105**, 433 (1955).
[20] V. A. Marchenko, Doklady Akad. Nauk S.S.S.R. **104**, 433 (1955).
[21] I. Kay and H. E. Moses, Nuovo cimento **2**, 917 (1955).
[22] I. Kay and H. E. Moses, Nuovo cimento **3**, 67 (1956).
[23] I. Kay and H. E. Moses, Nuovo cimento **3**, 277 (1956).
[24] I. Kay and H. E. Moses, Nuovo cimento Suppl. **5**, 230 (1957).
[25] K. O. Friedrichs, Math. Ann. **115**, 249 (1938).
[26] K. O. Friedrichs, Communs. Pure and Appl. Math. **1**, 361 (1948).
[27] R. G. Newton, Phys. Rev. **105**, 763 (1957).
[28] R. G. Newton, Phys. Rev. **107**, 1025 (1957).
[29] T. Fulton and R. G. Newton, Phys. Rev. **107**, 1102 (1957).

proof will be carried out in a completely rigorous fashion. Many of our considerations will be of a heuristic nature whenever the justification of details requires greater means than in other more standard proofs. We shall nevertheless use these heuristic proofs to avoid obscuring the conceptual side of the work with lengthy mathematical discussions. We are confident that the physicist will find our reasoning completely convincing and that the mathematician will be able to reconstruct the deficient proofs so as to make them completely rigorous. On the other hand, we have tried to state theorems in their most precise form.

Let us give a brief outline of the basic ideas and plan of the survey. The first 13 sections are devoted to the solution of the inverse-scattering problem for the operator L defined by Eq. (0.13) for $l = 0$ and the condition $\psi(0) = 0$. We consider L to be a perturbation of the operator L_0 defined by the differential expression $L_0\psi = -d^2\psi(x)/dx^2$ and the same condition $\psi(0) = 0$. According to Friedrichs, a transformation operator U is defined as the solution of the operator equation

$$LU = UL_0, \tag{0.14}$$

so that any transformation operator which has an inverse generates a similarity transformation of the the perturbed operator into the unperturbed:

$$U^{-1}LU = L_0. \tag{0.15}$$

The transformation operator U replaces the eigenfunctions of the continuous spectrum of L in all considerations. Roughly speaking, its kernel is obtained by expanding the eigenfunctions of the continuous spectrum of L in terms of the eigenfunctions of L_0.

In Secs. 4 and 5, it is shown that such transformation operators exist for our example and that the completeness theorem for the eigenfunctions of L, proved in Sec. 2, can be written in terms of a transformation operator in the form

$$UWU^* = I, \tag{0.16}$$

(for simplicity, we have restricted ourselves here to the case where L has no discrete spectrum; in the text, this restriction is not imposed). Here, W is a positive-definite self-adjoint operator commuting with L_0. W determines the "normalization" of the corresponding operator U.

A characteristic feature of our example is that among the transformation operators there exist Volterra operators of the form[30]

$$U_Bf(x) = (I + K)f(x) = f(x) + \int_0^x K(x, y)f(y)\,dy. \tag{0.17}$$

The operator W corresponding to U_B is constructed using

$$W(k) = 1/[M(k)M(-k)], \tag{0.18}$$

where $M(k)$ is a certain function introduced in Sec. 1. One might call $M(\lambda^{1/2})$ the determinant of the operator $L - \lambda I$. In fact, in Sec. 2 it is shown that this function appears in the denominator of the resolvent kernel of L and determines its singularities. These consist of a branch cut corresponding to the continuous spectrum and poles at the points of the discrete spectrum.

In Sec. 3, it is shown that the time-dependent formulation of the scattering problem is valid for our example provided that L_0 is taken to be the energy operator of the free particles and the corresponding scattering operator is defined by

$$S(k) = M(-k)/M(k). \tag{0.19}$$

In Sec. 6, it is shown how to establish the relationship between $W(k)$ and $S(k)$ with the help of (0.18) and (0.19).

In Sec. 8, on the basis of the triangularity of the kernel $K(x, y)$, a linear integral equation is obtained from (0.16) connecting the kernels of the operators W and K. In Sec. 9, this equation is studied and the inverse problem is solved for the case in which L has no discrete spectrum. Supplementary facts necessary for a treatment of the general case are cited in Sec. 12.

The approach described corresponds to the Gel'fand-Levitan method. Another procedure, related to Marchenko's method, is based on the application of the operator $V_B = I + A$ introduced in Secs. 4 and 7:

$$V_Bf(x) = f(x) + \int_x^\infty A(x, y)f(y)\,dy. \tag{0.20}$$

This operator is not a transformation operator in the general sense. However, its relation to the transformation operator $\tilde{U}_B = U_BW = (U_B^*)^{-1}$ is established in Sec. 7. This relation and (0.16) are then used to show that V_B satisfies the identity

$$V_B(I - F)V_B^* = I, \tag{0.21}$$

where the operator F can be constructed directly in terms of the function $S(k)$. By means of (0.21), a linear integral equation is deduced which relates the kernel $A(x, y)$ to the function $S(k)$, thus per-

[30] The subscript B used throughout and which transliterates into English as V stands, of course, for Volterra.

mitting one to solve the inverse problem. This integral equation is used in Sec. 10 to investigate the connection between $S(k)$ and $q(x)$. Several aspects of Krein's method are illustrated in Sec. 11. In Sec. 13, the construction of an operator L from a known operator L_1, when the S function of L differs from that of L_1 by a rational factor, is considered. This is important in applications. In Secs. 14 and 15, the results deduced are extended to the radial equation (0.13) where $l > 0$.

In order not to interrupt the presentation, we shall not mention original papers in the text. The literature is cited in a special Appendix. A number of comments are made there and a brief review is given of work done on the inverse scattering problem that has not been included in the text.

1. THE SOLUTIONS $\varphi(x, s)$, $f(x, s)$ AND THEIR RELATIONSHIP; EXISTENCE AND INEQUALITIES. THE FUNCTION $M(s)$ AND ITS PROPERTIES

In this section, some basic properties of solutions of the equation

$$-y'' + q(x)y = s^2 y, \qquad s = \sigma + i\tau \tag{1.1}$$

are assembled which will be utilized in the subsequent presentation. In all lemmas, it is assumed without further mention that $q(x)$ is a locally summable function and satisfies the condition

$$\int_0^\infty x\,|q(x)|\,dx = C < \infty. \tag{1.2}$$

The solutions $\varphi(x, s)$ and $f(x, s)$ are determined by the conditions:

$$\varphi(x, s):\ \varphi(0, s) = 0, \qquad \varphi'(0, s) = 1, \tag{1.3}$$

$$f(x, s):\ \lim_{x\to\infty} e^{-isx} f(x, s) = 1. \tag{1.4}$$

Equation (1.1) and the conditions (1.3) and (1.4) are equivalent to the following integral equations:

$$\varphi(x, s) = \frac{\sin sx}{s} + \int_0^x \frac{\sin s(x-t)}{s}\, q(t)\varphi(t, s)\,dt, \tag{1.5}$$

$$f(x, s) = e^{isx} + \int_x^\infty \frac{\sin s(t-x)}{s}\, q(t) f(t, s)\,dt, \tag{1.6}$$

which can be obtained by the method of variation of parameters. With the help of these equations the following lemmas are proven:

Lemma 1.1. *For each $x \geq 0$, $\varphi(x, s)$ is an entire function of s for which the estimate*[31]

$$|\varphi(x, s)| \leq Kxe^{|\tau|x}/(1 + |s|\,x) \tag{1.7}$$

holds. Moreover, $\varphi(x, s)$ is an even function of s for real s.

Lemma 1.2. *For each $x \geq 0$, $f(x, s)$ is analytic in s in the half-plane $\tau > 0$ and continuous down to the real axis. Moreover, the inequality*

$$|f(x, s)| \leq Ke^{-\tau x}, \qquad \tau \geq 0 \tag{1.8}$$

holds.

Lemma 1.3. *$f(x, s)$ satisfies the following inequalities:*

$$|f(x, s) - e^{isx}| \leq K\frac{e^{-\tau x}}{|s|}\int_x^\infty |q(t)|\,dt, \qquad \tau \geq 0, \tag{1.9}$$

$$|f(x, s) - e^{isx}| \leq Ke^{-\tau x}\int_x^\infty t\,|q(t)|\,dt, \qquad \tau \geq 0, \tag{1.10}$$

$$|f'(x, s) - ise^{isx}| \leq Ke^{-\tau x}\int_x^\infty |q(t)|\,dt, \qquad \tau \geq 0. \tag{1.11}$$

The estimate (1.9) is suitable for $|s| \to \infty$ and may be applied when $x \neq 0$. The estimates (1.10) and (1.11) are suitable for $x \to \infty$. In addition, (1.11) implies that

$$\lim_{x\to 0} xf'(x, s) = 0. \tag{1.12}$$

In fact, as $x \to 0$,

$$x\int_x^\infty |q(t)|\,dt \leq \int_x^{x^{1/2}} t\,|q(t)|\,dt + x^{1/2}\int_{x^{1/2}}^\infty t\,|q(t)|\,dt \to 0.$$

Lemma 1.4. *For any x, the function $f(x, s)$ is continuously differentiable with respect to s down to the line $\tau = 0$ with the possible exception of the point $s = 0$. The estimate*[32]

$$|\dot{f}(x, s) - ixe^{isx}| \leq \frac{K}{|s|}e^{-\tau x}, \qquad \tau \geq 0, \tag{1.13}$$

holds uniformly in x.

Lemma 1.5. *For large $|s|$*

$$\varphi(x, s) = \sin sx/s + o(e^{|\tau|x}/|s|), \tag{1.14}$$

$$f(x, s) = e^{isx} + o(e^{-\tau x}), \qquad \tau \geq 0, \tag{1.15}$$

uniformly for all $x \geq 0$.

When s is real, it is not difficult to establish a

[31] Absolute constants depending only on C (which may be different) will be denoted by K.

[32] The dot denotes differentiation with respect to s; a bar will denote complex conjugate.

relationship between $\varphi(x, s)$ and $f(x, s)$. Without further mention, we shall write k for s whenever s is real. The solutions $f(x, k)$ and $f(x, -k) = \bar{f}(x, k)$ for $k \neq 0$ are linearly independent solutions of Eq. (1.1). In fact, their Wronskian does not vanish:

$$[f(x, k); f(x, -k)] = f'(x, k)f(x, -k) - f(x, k)f'(x, -k) = 2ik. \quad (1.16)$$

In consequence of the realness of $\varphi(x, k)$

$$\varphi(x, k) = (1/2ik)[f(x, k)\overline{M}(k) - f(x, -k)M(k)], \quad (1.17)$$

where $M(k)$ may be found by the use of the Wronskian [see (1.12)]:

$$M(k) = [\varphi(x, k); f(x, k)] = \lim_{x\to 0} [\varphi(x, k); f(x, k)] = f(0, k). \quad (1.18)$$

From this and Lemma 1.2, we conclude that $M(k)$ is the limit of the function $M(s) = f(0, s)$, analytic in the upper half-plane, and is such that $M(k) = \bar{M}(-k)$. Let us introduce the notations

$$A(k) = |M(k)|, \qquad \eta(k) = \arg M(k), \quad (1.19)$$

so that

$$A(k) = A(-k), \qquad \eta(k) = -\eta(-k). \quad (1.20)$$

By Lemma 1.3 and (1.17), we infer that for large x

$$\varphi(x, k) = [A(k)/k] \sin [kx - \eta(k)] + o(1), \quad (1.21)$$

$$\varphi'(x, k) = A(k) \cos [kx - \eta(k)] + o(1). \quad (1.22)$$

It is therefore natural to call $A(k)$ the asymptotic *amplitude* and $\eta(k)$ the asymptotic *phase*.

Let $\tau > 0$. From Eq. (1.1) for $f(x, s)$ and the equation

$$-\dot{f}''(x, s) + q(x)\dot{f}(x, s) = 2sf(x, s) + s^2\dot{f}(x, s) \quad (1.23)$$

for $\dot{f}(x, s) = df(x, s)/ds$, it is not difficult to obtain the following identities:

$$f'(0, s)\bar{\dot{f}}(0, s) - f(0, s)\bar{\dot{f}}'(0, s) = 4i\sigma\tau \int_0^\infty |f(t, s)|^2\, dt, \quad (1.24)$$

$$\dot{f}'(0, s)f(0, s) - \dot{f}(0, s)f'(0, s) = 2s \int_0^\infty f^2(t, s)\, dt. \quad (1.25)$$

From the first one, we conclude that $M(s)$ can vanish only for $\sigma = 0$ or $\tau = 0$. The second possibility, however, is excluded by the fact that if $M(k) = 0$ on the real axis, (1.17) would imply that $\varphi(x, k) \equiv 0$, and this is impossible.

In the following, it will be assumed that $M(0) \neq 0$. The vanishing of $M(s)$ for $s = 0$ is equivalent to the solution of $-y'' + q(x)y = 0$, $y(0) = 0$ being bounded as $x \to \infty$ and this happens only in exceptional situations. A treatment of the case $M(0) = 0$ presents no essential difficulties but only encumbers the formulation and proof of theorems.

There still remains the possibility that $M(s) = 0$ for $\sigma = 0$ and $\tau > 0$. From the estimate

$$M(s) = 1 + o(1) \quad (1.26)$$

for large $|s|$, which follows from formula (1.15), we conclude that $M(s)$ can only have a finite number of zeros $s_n = i\kappa_n$ $(n = 1, \cdots, m)$ on the imaginary axis. When $s = s_n$, the solutions $\varphi(x, s_n)$ and $f(x, s_n)$ satisfy the same boundary condition at $x = 0$, and are therefore proportional:

$$f(x, s_n) = f'(0, s_n)\varphi(x, s_n). \quad (1.27)$$

From this and (1.25), it follows that

$$\int_0^\infty [\varphi(x, s_n)]^2\, dx = -\frac{\dot{M}(s_n)}{2s_n f'(0, s_n)}, \quad (1.28)$$

and this implies, in particular, that $M(s)$ has only simple zeros. The above results can be formulated as follows.

Lemma 1.6. *The function $M(s)$ is analytic in the upper half-plane and has there a finite number of simple zeros $s_n = i\kappa_n$, $\kappa_n > 0$, $(n = 1, \cdots, m)$. For large $|s|$, the estimate* (1.26) *holds. The function $\dot{M}(s)$ is continuous down to the real axis with the possible exception of the point $s = 0$. Furthermore, $s\dot{M}(s)$ is continuous everywhere in the half-plane* $\operatorname{Im} s \geq 0$.

The two last assertions follow from Lemma 1.4.

2. EXPANSION THEOREM

The differential equation (1.1) together with the boundary condition, defines a self-adjoint operator in $\mathfrak{L}_2(0, \infty)$. This operator can be obtained by the extension of the symmetric operator, defined by (1.1), acting on the twice-continuously differentiable functions satisfying the boundary condition and vanishing identically outside some finite interval. We shall denote this operator by L.

Consider the kernel

$$\left.\begin{aligned} R_\lambda(x, y) &= \varphi(x, \lambda^{1/2})f(y, \lambda^{1/2})/M(\lambda^{1/2}), \quad x < y, \\ R_\lambda(x, y) &= R_\lambda(y, x), \\ 0 &\leq \arg \lambda^{1/2} \leq \pi, \end{aligned}\right\} \quad (2.1)$$

which is defined for all complex λ with the exception of a finite number of points on the negative real axis corresponding to the zeros of $M(\lambda^{1/2})$. By virtue of (1.18), it is not difficult to verify that the kernel $R_\lambda(x, y)$ is a solution of the equation

$$(-d^2/dx^2 + q(x))R_\lambda(x, y) - \lambda R_\lambda(x, y) = \delta(x - y), \tag{2.2}$$

and satisfies the boundary conditions

$$R_\lambda(0, y) = R_\lambda(x, 0) = 0. \tag{2.3}$$

In consequence of (1.7) and (1.8), we have

$$|R_\lambda(x, y)| \leq K \frac{x}{1 + |\lambda^{1/2}|\, x} e^{-\tau|x-y|}, \qquad \tau = \operatorname{Im} \lambda^{1/2} > 0 \tag{2.4}$$

for complex λ and, hence, the kernel $R_\lambda(x, y)$ defines a bounded operator in $\mathfrak{L}_2(0, \infty)$, namely, the resolvent operator

$$R_\lambda = (L - \lambda I)^{-1}. \tag{2.5}$$

The singularities of R_λ in the complex λ plane consist of a cut along the positive real axis and a finite number of simple poles $\lambda_n = -\kappa_n^2$ $(n = 1, \cdots, m)$ on the negative real axis. The continuous and discrete portions of the spectrum correspond to the cut and poles, respectively. The jump in the resolvent across the cut and the residues at the poles determine the spectral function of the operator L. We come now to the following completeness theorem for the eigenfunctions of the operator L.

Theorem 2.1. *The functions* $\varphi(s, k)$ $(k \geq 0)$ *and* $\varphi_n(x) = \varphi(x, i\kappa_n)$ *form a complete orthogonal system. The completeness relationship is given by*

$$\sum_{n=1}^{m} C_n \varphi_n(x)\varphi_n(y) + \frac{2}{\pi}\int_0^\infty \varphi(x, k) \frac{1}{M(k)M(-k)} \times \varphi(y, k)k^2\, dk = \delta(x - y), \tag{2.6}$$

in which $C_n = 2i\kappa_n f'(0, i\kappa_n)/\dot{M}(i\kappa_n)$ [*see* (1.28)].

Formula (2.6) can be deduced without recourse to general operator theory. Let $f(x)$ be a twice-continuously differentiable function vanishing for large x and in the neighborhood of $x = 0$. Then

$$g(x) = -f''(x) + q(x)f(x) \tag{2.7}$$

is continuous and vanishes identically outside some finite interval not containing the origin. From (2.2) and (2.7), it follows that

$$\int_0^\infty R_\lambda(x, y)f(y)\, dy = -\frac{1}{\lambda} f(x) + \frac{1}{\lambda}\int_0^\infty R_\lambda(x, y)g(y)\, dy. \tag{2.8}$$

If we integrate both sides of (2.8) around a large circle $|\lambda| = N$, then the contribution from the second term on the right-hand side of (2.8) will approach zero as $N \to \infty$ by virtue of (1.14), (1.15), and (1.26). Thus we have

$$\lim_{N\to\infty} \frac{1}{2\pi i} \oint_{\lambda=|N|} \left[\int_0^\infty R_\lambda(x, y)f(y)\, dy\right] d\lambda = -f(x). \tag{2.9}$$

On the other hand, if we integrate the left-hand side of (2.8) along a path γ consisting of a curve encompassing the cut on the real axis and a large circle $|\lambda| = N$, we obtain

$$\frac{1}{2\pi i}\oint_\gamma \left\{\int_0^\infty R_\lambda(x, y)f(y)\, dy\right\} d\lambda = \frac{1}{2\pi i}\oint_{|\lambda|=N} \left\{\int_0^\infty R_\lambda(x, y)f(y)\, dy\right\} d\lambda + \frac{1}{2\pi i}\int_0^\infty d\sigma\left\{\int_0^\infty [R_{\sigma+i0}(x, y) - R_{\sigma-i0}(x, y)]f(y)\, dy\right\} = \sum_{n=1}^{m} \operatorname{res}\left\{\int_0^\infty R_\lambda(x, y)f(y)\, dy\right\}\Big|_{\lambda=\lambda_n}.$$

Taking into consideration (2.1) and (1.17) and letting $N \to \infty$, we find, on the basis of (2.9), that

$$f(x) = \frac{2}{\pi}\int_0^\infty k^2\, dk \times \left\{\int_0^\infty \varphi(x, k) \frac{1}{M(k)M(-k)} \varphi(y, k)f(y)\, dy\right\} + \sum_{n=1}^{m}\int_0^\infty C_n\varphi_n(x)\varphi_n(y)f(y)\, dy.$$

Finally, by virtue of the fact that the functions $f(x)$ are dense in $\mathfrak{L}_2(0, \infty)$, formula (2.6) is obtained.

The functions $\psi^{(+)}(x, k) = \varphi(x, k)/M(k)$ and $\psi_n(x) = C_n^{1/2}\, \varphi_n(x)$ form an orthonormal system. However, the functions $\psi^{(+)}(x, k)$ are not square integrable, and hence, are not elements of Hilbert space nor eigenfunctions in the usual sense. To attach meaning to them while still remaining in the framework of Hilbert space, we may consider them to be kernels of transformations which diagonalize the operator L. Thus, the transformation

$$T^{(+)}g = G: \quad G(k) = \int_0^\infty g(x)\psi^{(+)}(x, k)\, dx \tag{2.10}$$

carries any function $g(x)$ in $\mathfrak{L}_2(0, \infty)$ into a function $G(k)$ for which $\int_0^\infty |G(k)|^2\, k^2\, dk < \infty$. Moreover, if $Lg(x)$ belongs to $\mathfrak{L}_2(0, \infty)$, then $Lg(x)$ goes into $k^2G(k)$, and the integral $\int_0^\infty |G(k)k^2|\, k^2\, dk$ exists. In the following, the space of functions $G(k)$ with

the scalar product

$$(G, G_1) = \frac{2}{\pi}\int_0^\infty \bar{G}(k)G_1(k)k^2\,dk \qquad (2.11)$$

will be denoted by $\mathfrak{L}_k$, and the space of square integrable functions $g(x)$, which was previously called $\mathfrak{L}_2(0, \infty)$, will be denoted by $\mathfrak{L}_x$. The transformation $T^{(+)}$ acts from $\mathfrak{L}_x$ into $\mathfrak{L}_k$. The adjoint transformation $T^{(+)*}$ acts from $\mathfrak{L}_k$ into $\mathfrak{L}_x$ according to the formula

$$g = T^{(+)*}G\colon\ g(x) = \frac{2}{\pi}\int_0^\infty G(k)\bar{\psi}^{(+)}(x, k)k^2\,dk. \qquad (2.12)$$

The orthogonality of the eigenfunctions $\psi^{(+)}(x, k)$ can thus be expressed in these new terms as follows:

$$T^{(+)}T^{(+)*} = I^k. \qquad (2.13)$$

Here, I^k denotes the identity operator in L_k. The formula (2.6) can now be written in the following form:

$$T^{(+)*}T^{(+)} = I_c^x. \qquad (2.14)$$

Here, I_c^x is a projection onto the proper subspace of the operator L corresponding to its continuous spectrum. The superscript x indicates that this operator acts on $\mathfrak{L}_x$. A transformation such as $T^{(+)}$ can be associated with any solution of Eq. (1.1) satisfying a zero boundary condition. Let $\chi(x, k)$ be a solution of (1.1) such that $\chi(0, k) = 0$ and $\chi'(0, k) \neq 0$ for all k. Consider the transformation

$$Tg = G\colon\quad G(k) = \int_0^\infty g(x)\chi(x, k)\,dx. \qquad (2.15)$$

The transformations T and $T^{(+)}$ are related by the formula

$$T = N^kT^{(+)}, \qquad (2.16)$$

where N^k is a 'normalizing factor'; N^k is an operator in $\mathfrak{L}_k$, which multiplies by the function $N(k) = \chi'(0, k)/\psi^{(+)\prime}(0, k)$. The completeness relation and orthogonality condition can be written in terms of T as follows:

$$T^*W^kT = I_c^x, \qquad TT^*W^k = I^k, \qquad (2.17)$$

where

$$W^k = (N^{k*})^{-1}(N^k)^{-1}. \qquad (2.18)$$

The somewhat formal reasoning used at the end of this section will turn out to be useful in Sec. 5.

3. ASYMPTOTIC BEHAVIOR OF THE SOLUTION OF THE SHRÖDINGER EQUATION FOR LARGE TIME

The expansion theorem for the eigenfunctions of the operator L deduced in the preceding section enables us to use Fourier methods to solve time-dependent equations involving the operator L. We shall be particularly interested in the behavior of solutions of the Schrödinger equation

$$i\,\partial f(x, t)/\partial t = Lf(x, t),\quad f(x, t)\,|_{t=0} = f_0(x) \qquad (3.1)$$

for large $|t|$.

By expanding $f_0(x)$ in terms of the eigenfunctions of L, we can represent the solution of (3.1) in the following way:

$$f(x, t) = \frac{2}{\pi}\int_0^\infty F(k)\bar{\psi}(x, k)e^{-ik^2t}k^2\,dk + \sum_{n=1}^{m} F_n\bar{\psi}_n(x)e^{i\kappa_n^2t}. \qquad (3.2)$$

Here, $\psi(x, k)$ and $\psi_n(x)$ comprise any orthonormal system of eigenfunctions of L [$\psi(x, k)$ and $\psi_n(x)$ may differ from the functions $\psi^{(+)}(x, k)$ and $\psi_n(x)$ discussed in Sec. 2 by a factor of modulus 1] and

$$F(k) = \int_0^\infty f_0(x)\psi(x, k)\,dx,\ F_n = \int_0^\infty f_0(x)\psi_n(x)\,dx. \qquad (3.3)$$

In particular, one may take as the set $\psi(x, k)$ the functions $\psi^{(+)}(x, k)$ or

$$\psi^{(-)}(x, k) = \psi^{(+)}(x, k)M(k)/M(-k) = \bar{\psi}^{(+)}(x, k).$$

The behavior of $f(x, t)$ for large $|t|$ can be analyzed on the basis of the following lemma:

Lemma 3.1. *Let $F(k)$ be an arbitrary function of $\mathfrak{L}_k$, i.e.,*

$$\int_0^\infty |F(k)|^2\,k^2\,dk < \infty, \qquad (3.4)$$

and set

$$f^{(\pm)}(x, t) = \int_0^\infty F(k)\bar{\psi}^{(\pm)}(x, k)e^{-ik^2t}k^2\,dk, \qquad (3.5)$$

$$g(x, t) = \int_0^\infty F(k)\frac{\sin kx}{k}e^{-ik^2t}k^2\,dk. \qquad (3.6)$$

Then

$$\lim_{t\to\pm\infty}\int_0^\infty |f^{(\pm)}(x, t) - g(x, t)|^2\,dx = 0. \qquad (3.7)$$

It is sufficient to prove the statement for a set of functions $F(k)$ which is dense in $\mathfrak{L}_k$; the theorem then follows for any function by completion. We assume that $F(k)$ is differentiable and nonvanishing only in the interval $0 < \alpha \leq k \leq \beta < \infty$. The intervals of integration in (3.5) and (3.6) are then finite and do not contain the point $k = 0$. For

definiteness, we shall suppose that $t \to \infty$. By virtue of the fact that $\psi^{(+)}(x, k)$ and $(\sin kx)/k$ are uniformly bounded for x in $0 < x < \infty$ and k in $[\alpha, \beta]$, the functions $f^{(+)}(x, t)$ and $g(x, t)$ tend to zero as $t \to \infty$ uniformly in x. Thus the integral in (3.7) vanishes as $t \to \infty$ for any finite interval of integration. We still have to show that $\int_A^\infty |f^{(+)} - g|^2\, dx$ converges for arbitrary A.

From (1.17) and the definition of $\psi^{(+)}(x, k)$,

$$\psi^{(+)}(x, k) - \frac{\sin kx}{k} = -\frac{1}{2ik} e^{-ikx}\left[\frac{M(k)}{M(-k)} - 1\right] + R(x, k), \tag{3.8}$$

where for $x > 0$

$$|R(x, k)| \leq K \frac{1}{k^2} \int_x^\infty |q(t)|\, dt \tag{3.9}$$

by virtue of (1.9) and (1.8). In consequence of this estimate,

$$\int_A^\infty \left| \int_\alpha^\infty F(k) R(x, k) e^{-ik^2 t} k^2\, dk \right|^2 dx \leq K \int_A^\infty dx \left(\int_x^\infty |q(t)|\, dt \right)^2 \int_\alpha^\infty |F(k)|^2 k^2\, dk \int_\alpha^\infty \frac{dk}{k^2} \leq K' \int_A^\infty |q(t)|\, dt \int_A^\infty t\, |q(t)|\, dt, \tag{3.10}$$

and for sufficiently large A the integral containing $R(x, k)$ can be made as small as desired uniformly in t. We must still look at the behavior of the integral of the basic term of (3.8)

$$Q_A(t) = \int_A^\infty dx \left| \int_\alpha^\infty G(k) e^{-ikx} e^{-ik^2 t}\, dk \right|^2, \tag{3.11}$$

as $t \to \infty$. The function

$$G(k) = \frac{F(k)}{2ik}\left[\frac{M(k)}{M(-k)} - 1\right] k^2$$

is finite and continuously differentiable by Lemma 1.6. Now $Q_A(t) = \lim_{B \to \infty} Q_A^B(t)$ where

$$Q_A^B(t) = \int_A^B dx \left| \int_\alpha^\beta G(k) e^{-ikx} e^{-ik^2 t}\, dk \right|^2 = \int_\alpha^\beta dk \int_\alpha^\beta dl \left\{ G(k) \overline{G}(l) e^{-i(k^2 - l^2)t} \times \frac{e^{-i(k-l)A} - e^{-i(k-l)B}}{i(k - l)} \right\} = J_A(t) - J_B(t).$$

Here

$$J_B(t) = \int_\alpha^\beta dk \int_\alpha^\beta dl G(k) \overline{G}(l) \frac{e^{-i(k^2 - l^2)t} e^{-i(k-l)B}}{i(k - l)}.$$

Because of the singularity in the denominator, the inner integral is understood to be a principal-valued integral, defined in consequence of the differentiability of $G(k)$.

We now transform $J_B(k)$ as follows:

$$J_B(t) = \int_\alpha^\beta dk G(k) \times \left[\int_\alpha^\beta dl \frac{\overline{G}(l) e^{-i(k^2 - l^2)t} - \overline{G}(k)}{i(k - l)} e^{-i(k-l)B} + \overline{G}(k) \int_\alpha^\beta \frac{e^{-i(k-l)B}}{i(k - l)} dl \right]. \tag{3.12}$$

The first term in the integral with respect to l is continuous for $k = l$, and hence, vanishes as $B \to \infty$ by the Riemann-Lebesgue theorem. The second term in this integral tends to π as $B \to \infty$, and therefore, we find that $\lim_{B \to \infty} J_B(t)$ is independent of t and has the value

$$\pi \int_\alpha^\beta |G(k)|^2\, dk.$$

$J_A(t)$ can also be represented as the sum of two terms, one vanishing as $t \to \infty$ uniformly in A, and the other having a finite limit independent of A as $t \to \infty$ equal to $\pi \int_\alpha^\beta |G(k)|^2\, dk$. From this it follows that $Q_A(t) \to 0$ and the lemma is therefore proven.

Let us now return to the investigation of the behavior of the solution $f(x, t)$ of the Schrödinger equation. If $f_0(x)$ is orthogonal to the eigenfunctions of the discrete spectrum of L, then the sum in the second term of (3.2) does not appear. Let

$$F^{(-)}(k) = \int_0^\infty f_0(x) \psi^{(-)}(x, k)\, dx. \tag{3.13}$$

These are the functions which occur in formula (3.2) for $f(x, t)$, $\psi^{(-)}(x, k)$ having been selected instead of $\psi(x, k)$. Clearly,

$$g^{(-)}(x, t) = \frac{2}{\pi} \int_0^\infty F^{(-)}(k) \frac{\sin kx}{k} e^{-ik^2 t} k^2\, dk \tag{3.14}$$

is a solution of the Schrödinger equation with an operator L_0 associated with the equation $L_0 y = -y'' = k^2 y$ and the boundary condition $y(0) = 0$, i.e.,

$$i\, \partial g^{(-)}(x, t)/\partial t = L_0 g^{(-)}(x, t), \tag{3.15}$$

where

$$g^{(-)}(x, 0) = g_0^{(-)}(x) = \frac{2}{\pi} \int_0^\infty F^{(-)}(k) \frac{\sin kx}{k} k^2\, dk. \tag{3.16}$$

If, in analogy with Sec. 2, we introduce a unitary transformation T_0 of $\mathfrak{L}_x$ into $\mathfrak{L}_k$ given by

$$T_0 g = G: \quad G(k) = \int_0^\infty g(x) \frac{\sin kx}{k}\, dx, \tag{3.17}$$

then $g_0^{(*)}(x)$ can be expressed in terms of $f_0(x)$ by the formula

$$g_0^{(*)}(x) = T_0^* T^{(*)} f_0(x). \tag{3.18}$$

From Lemma 3.1 follows Theorem 3.1.

Theorem 3.1. *If $f_0(x)$ is orthogonal to the eigenfunctions of the discrete spectrum of L, then when $t \to \pm\infty$ the solution of the Schrödinger equation* (3.1) *behaves like the solution of the Schrödinger equation* (3.15) *with initial data $g_0^{(*)}(x)$ given by* (3.18), *in the sense that*

$$\int_0^\infty |f(x, t) - g^{(*)}(x, t)|^2\, dx \to 0 \text{ as } t \to \pm\infty. \tag{3.19}$$

4. TRANSFORMATION OPERATORS

In the following we shall need the representation of a solution of (1.1) with a potential $q(x)$ in terms of solutions of the equation with other potentials and, in particular, with $q(x) \equiv 0$, i.e., in terms of trigonometric functions.

The simplest such expression can be deduced in the following way. On the basis of (1.9) for $x \neq 0$, the function $h(x, s) = f(x, s) - e^{isx}$ is square integrable in s along any line parallel to the real axis, and in the upper half-plane

$$\int_{-\infty}^\infty |h(x, \sigma + i\tau)|^2\, d\sigma = O(e^{-2\tau x}).$$

By a theorem of Titchmarsh,

$$A(x, y) = \frac{1}{2\pi} \int_{-\infty}^\infty [f(x, k) - e^{ikx}] e^{-iky}\, dk = 0, \quad x > y. \tag{4.1}$$

The inversion of this Fourier transform thus yields

$$f(x, s) = e^{isx} + \int_x^\infty A(x, y) e^{isy}\, dy, \quad \tau \geq 0, \tag{4.2}$$

where $A(x, y)$ is square integrable in y for $x \neq 0$. With certain modifications, this procedure yields an expression for $\varphi(x, s)$ valid for all s:

$$\varphi(x, s) = \frac{\sin sx}{s} + \int_0^x K(x, y) \frac{\sin sy}{s}\, dy. \tag{4.3}$$

However, the derivation gives almost no information concerning the kernels $K(x, y)$ and $A(x, y)$. Equivalent equations for these kernels can be deduced by substituting expressions (4.2) and (4.3) for $f(x, s)$ and $\varphi(x, s)$ into (1.6) and (1.5), respectively, and by eliminating the trigonometric functions. This yields

$$K(x, y) = \frac{1}{2} \int_{(x-y)/2}^{(x+y)/2} q(t)\, dt + \int_{(x-y)/2}^{(x+y)/2} dt \times \int_0^{(x-y)/2} dz q(t + z) K(t + z, t - z), \quad x \geq y, \tag{4.4}$$

$$A(x, y) = \frac{1}{2} \int_{(x+y)/2}^\infty q(t)\, dt - \int_{(x+y)/2}^\infty dt \times \int_0^{(y-x)/2} dz q(t - z) A(t - z, t + z), \quad y \geq x. \tag{4.5}$$

By then solving these equations by the method of successive approximations, we obtain estimates for $K(x, y)$ and $A(x, y)$:

$$|K(x, y)| \leq \frac{1}{2} \int_{(x-y)/2}^x |q(t)|\, dt \times \exp \int_0^{(x+y)/2} t\, |q(t)|\, dt, \tag{4.6}$$

$$|A(x, y)| \leq \frac{1}{2} \int_{(x+y)/2}^\infty |q(t)|\, dt \times \exp \int_x^\infty t\, |q(t)|\, dt. \tag{4.7}$$

The above integral equations can also be used to show that $K(x, y)$ and $A(x, y)$ are differentiable and to derive estimates for their derivatives. For example,

$$\left| \frac{\partial}{\partial x} A(x, y) + \frac{1}{4} q\left(\frac{x + y}{2}\right) \right| \leq K \int_x^\infty |q(t)|\, dt \int_{(x+y)/2}^\infty |q(t)|\, dt. \tag{4.8}$$

A similar inequality holds for $\partial A(x, y)/\partial y$.

By virtue of (4.6) and (4.7), the theory of Volterra integral equations may be applied to integral equations having $K(x, y)$ and $A(x, y)$ as kernels. Thus, if $g(x)$ belongs to a given class of functions (which we shall not specify), then the equations

$$U_B f(x) \equiv f(x) + \int_0^x K(x, y) f(y)\, dy = g(x), \tag{4.9}$$

$$V_B f(x) \equiv f(x) + \int_x^\infty A(x, y) f(y)\, dy = g(x) \tag{4.10}$$

have solutions which may be represented in the form

$$f(x) = g(x) + \int_0^x \tilde{K}(x, y) g(y)\, dy \equiv U_B^{-1} g(x), \tag{4.11}$$

$$f(x) = g(x) + \int_x^\infty \tilde{A}(x, y)g(y)\,dy \equiv V_B^{-1}g(x). \quad (4.12)$$

In connection with this, the kernels $\tilde{K}(x, y)$ and $\tilde{A}(x, y)$ have estimates similar to (4.6) and (4.7). A more precise definition of the operators U_B and V_B as operators in Hilbert space will be given in the subsequent sections.

Relationships analagous to (4.3) exist between any two solutions of (1.1) with different potentials. Let $\varphi_1(x, k)$ and $\varphi_2(x, k)$ be solutions of (1.1) with potentials $q_1(x)$ and $q_2(x)$, respectively; two relations such as (4.3) can then be derived:

$$\varphi_1(x, k) = U_B^{(1)} \sin(kx)/k,$$
$$\varphi_2(x, k) = U_B^{(2)} \sin(kx)/k. \quad (4.13)$$

Inverting the second of these and substituting the result in the first, we obtain

$$\varphi_1(x, k) = U_B^{(1)}(U_B^{(2)})^{-1}\varphi_2(x,k) \quad (4.14)$$

or, explicitly,

$$\varphi_1(x, k) = \varphi_2(x, k) + \int_0^x K(x, y)\varphi_2(y, k)\,dy. \quad (4.15)$$

It is also possible to derive an inequality for $K(x, y)$ such as (4.6). Finally, one may also relate two different solutions $f_1(x, k)$ and $f_2(x, k)$, but such an expression will not be required in the following.

5. GENERAL THEORY OF TRANSFORMATION OPERATORS

We consider the operator L introduced in Sec. 2 to be one of the functional representations of an abstract operator, which will also be denoted by L. The operator L of Sec. 2 will now be denoted by L^x and the space $\mathfrak{L}_x$ in which it operates will be called the coordinate representation or x representation. Another representation to be considered is the so-called momentum or k representation. This space is of type $\mathfrak{L}_k$ and is defined by the condition that L_0 is an operator which multiplies an element of it by k^2:

$$L_0F(k) = k^2F(k). \quad (5.1)$$

Both representations are related to one another by the unitary transformation T_0 introduced in Sec. 3. In other words, to each element $f(x) \in \mathfrak{L}_x$, there corresponds an element $F(k)$ belonging to $\mathfrak{L}_k$:

$$F(k) = T_0f(x) = \int_0^\infty f(x)\frac{\sin kx}{k}\,dx; \quad (5.2)$$

and each operator A^x in $\mathfrak{L}_x$ is converted into an operator $A^k = T_0A^xT_0^*$. For example, in the k representation L is given by

$$L^kF(k) = k^2F(k) + \frac{2}{\pi}\int_0^\infty V(k, l)F(l)l^2\,dl, \quad (5.3)$$

where

$$V(k, l) = \int_0^\infty \frac{\sin kx}{k}\,q(x)\,\frac{\sin lx}{l}\,dx. \quad (5.4)$$

The passage back from the momentum to the coordinate representation is effected by the use of the transformation T_0^*; thus, for example, the operator which multiplies by a decreasing function $\Omega(k)$ goes into an integral operator in the x representation with a kernel

$$\Omega(x, y) = \frac{2}{\pi}\int_0^\infty \frac{\sin kx}{k}\,\Omega(k)\,\frac{\sin ky}{k}\,k^2\,dk. \quad (5.5)$$

In Sec. 2, the eigenfunction expansion theorem for L was expressed in terms of the operator T and involved various spaces. This is inconvenient. Instead of such transformations as T, we shall utilize operators acting in the same space, and which can therefore be prescribed by one of their representations. These operators are defined in the coordinate and momentum representations in the following way:

$$U^k = T_0T^* \text{ in the } k \text{ representation},$$
$$U^x = T^*T_0 \text{ in the } x \text{ representation}. \quad (5.6)$$

Such operators will be called transformation operators. In all subsequent discussions, they completely replace the eigenfunctions of the continuous spectrum. Instead of a differential equation for the eigenfunctions $\chi(x, k)$, one has for the operator U determined by them, the equation

$$LU = UL_0. \quad (5.7)$$

The completeness condition and orthogonality of the eigenfunctions in terms of U are expressed by

$$UWU^* = I_c, \qquad U^*UW = I \quad (5.8)$$

[cf. (2.17)]. The operator W in (5.8) is an operator which multiplies by the function $W(k)$ in the momentum representation. The advantage of (5.7) and (5.8) is that we do not have to write superscripts indicating the spaces in which the operators act—all operators are taken in the same representation. In many problems related to the operator L the use of different transformation operators is advantageous. Thus, the operators $U^{(*)}$ obtained from the transformations $T^{(*)}$ by means of (5.6) turn out to be useful in studying the asymptotic behavior of the solution of the Schrödinger equation

$$i\,\partial z(t)/\partial t = Lz(t), \qquad z(t)\,|_{t=0} = z_0 \quad (5.9)$$

for large $|t|$. The solution can be written in the following form:

$$z(t) = e^{-iLt}z_0, \tag{5.10}$$

and Theorem 3.1 can now be reformulated as follows.

Theorem 5.1. *If z_0 is orthogonal to the eigenfunctions of the point spectrum of L, then for the solution of the Schrödinger equation, the limiting conditions*

$$\lim_{t\to\pm\infty} e^{iL_0t}z(t) = z_\pm \tag{5.11}$$

hold where

$$z_+ = U^{(+)*}z_0, \qquad z_- = U^{(-)*}z_0. \tag{5.12}$$

If we denote the 'normalizing factor' relating $U^{(+)}$ and $U^{(-)}$ by S:

$$U^{(-)} = U^{(+)}S, \tag{5.13}$$

then (5.12) shows that z_+ and z_- are related to one another by

$$z_+ = Sz_-. \tag{5.14}$$

It is also not difficult to show from the definition of $U^{(+)}$ and (5.13) that in the momentum representation this is an operator which multiplies by the function

$$S(k) = M(-k)/M(k). \tag{5.15}$$

$S(k)$ obviously has the absolute value one. From Theorem 5.1 follows the existence of a solution of the Schrödinger equation which is asymptotic to the vector $z_-(t) = e^{-iL_0t}z_-$ as $t \to -\infty$, z_- being an arbitrary element. In addition, this solution for $t = 0$ will be orthogonal to the eigenfunctions of the point spectrum of L and consequently will behave like $e^{-iL_0t}z_+$ as $t \to \infty$, z_+ being constructed from (5.14) using the operator S. Thus, the general formulation of the scattering problem described in the introduction turns out to be valid for L, and S plays the role of the scattering operator. We have also shown that S is unitary and commutes with the energy operator.

The main objective of the survey is to establish the relationship between L and S. The operator $U_B = I + K$, defined in the coordinate representation by (4.9), will play an important role in this. By the definition of this section, this operator is a transformation operator. In fact, if we assume the transformation operator to be an integral operator, then its kernel in the x representation is obtained by expanding an appropriate solution $\chi(x, k)$ with respect to $(\sin kx)/k$:

$$\begin{aligned} U(x, y) &= \frac{2}{\pi}\int_0^\infty \chi(x, k)\frac{\sin ky}{k}k^2\,dk \\ &= \frac{2}{\pi}\int_0^\infty \left[\chi(x, k) - \frac{\sin kx}{k}\right] \\ &\quad \times \frac{\sin ky}{k}k^2\,dk + \delta(x - y). \end{aligned} \tag{5.16}$$

The kernel of the operator $U_B - I$ was derived in precisely this way in Sec. 4, where $\phi(x, k)$ is the corresponding solution. This crude argument can be put on an exact basis. In consequence of the fact that $M(k)$ is the normalizing factor for the solution $\varphi(x, k)$, with the help of which U_B is constructed, the operator W appearing in the formula for U_B, Eq. (5.8), is defined by

$$W(k) = 1/[M(k)M(-k)]. \tag{5.17}$$

A characteristic property of U_B is that it is a Volterra operator in the coordinate representation. This property is closely related to the fact that the potential $q(x)$ is diagonal in this representation (i.e., it is a multiplication operator). In fact, the triangularity of the kernel $K(x, y)$ is a consequence of the fact that $\varphi(x, s)$ is an entire function of s and this depends on the potential being diagonal. Conversely, let there exist a transformation operator U_B for some operator $L = L_0 + V$ of Volterra type in the x representation, namely,

$$U_B(x, y) = \delta(x - y) + \eta(x - y)K(x, y), \tag{5.18}$$

where

$$\eta(t) = \begin{matrix} 1 & \text{for} & t > 0 \\ 0 & \text{for} & t < 0. \end{matrix} \tag{5.19}$$

From (5.7), we find

$$V(I + K) = KL_0 - L_0K. \tag{5.20}$$

The operator $B = KL_0 - L_0K$ has the kernel

$$\begin{aligned} B(x, y) &= 2\,\delta(x - y)\,dK(x, x)/dx + \eta(x - y) \\ &\quad \times [\partial^2K(x, y)/\partial x^2 - \partial^2K(x, y)/\partial y^2]. \end{aligned} \tag{5.21}$$

Multiplying (5.20) by $(I + K)^{-1}$, we find, by (5.21), that

$$\begin{aligned} V(x, y) &= \delta(x - y)2\,dK(x, x)/dx \\ &\quad + \eta(x - y)C(x, y). \end{aligned} \tag{5.22}$$

But since V has to be self-adjoint,

$$C(x, y) = 0, \qquad V(x, y) = \delta(x - y)2\,dK(x, x)/dx, \tag{5.23}$$

i.e., L is defined by an equation of type (1.1). A

precise statement of the above conclusions is contained in the following theorem:

Theorem 5.2. *Let L_0 be an operator defined in the x representation by the differential expression $L_0y = -y''$ and the condition $y(0) = 0$. If there exists a self-adjoint operator $L = L_0 + V$ and Volterra operator $U_B = I + K$, whose kernel is differentiable and such that* (5.7) *is satisfied, then V is an operator which in the x representation, multiplies by the function*

$$q(x) = 2\,dK(x, x)/dx. \tag{5.24}$$

If the kernel of the transformation operator is not differentiable, then it is still possible to define L by the differential expression $Ly = -y'' + q(x)y$; but, in this case, $q(x)$ is a generalized function such as the derivative of an ordinary function. In particular, it is possible to obtain potentials with δ-function singularities.

Simultaneously with Theorem 5.2, we have shown that the kernel $K(x, y)$ satisfies the equation

$$q(x)K(x, y) = \partial^2K(x, y)/\partial x^2 - \partial^2K(x, y)/\partial y^2, \quad x > y. \tag{5.25}$$

In fact, by substituting (5.23) into the left-hand side and (5.21) into the right-hand side of (5.20), we obtain

$$q(x)\,\delta(x - y) + \eta(x - y)q(x)K(x, y) = q(x)\,\delta(x - y) + \eta(x - y)[\partial^2K(x, y)/\partial x^2 - \partial^2K(x, y)/\partial y^2], \tag{5.26}$$

and this implies Eq. (5.25). Of course, whenever its derivatives do not exist, then $K(x, y)$ is a generalized solution of this equation. On the basis of this equation for $K(x, y)$, the condition $K(x, 0) = 0$ [which follows directly from the definition of $K(x, y)$], and (5.24), it is not difficult to derive (4.4), already used earlier.

6. THE FUNCTIONS $W(k)$ AND $S(k)$, THEIR PROPERTIES AND RELATIONSHIP

In this section, we study the functions $W(k)$ and $S(k)$ which were introduced in the preceding section by

$$W(k) = 1/[M(k)M(-k)] \quad (-\infty < k < \infty), \tag{6.1}$$

$$S(k) = M(-k)/M(k) \quad (-\infty < k < \infty), \tag{6.2}$$

and we shall establish how they are related. In addition to the properties of $M(k)$ assembled in Lemma 1.6, we still require one further property:

Lemma 6.1. *$M(k)$ has the representation*

$$M(k) = 1 + \int_0^\infty \Gamma(t)e^{ikt}\,dt, \tag{6.3}$$

where $|\Gamma(t)|$ is integrable.

The proof follows immediately from the definition of $M(k)$ and the expression (4.2). These imply that

$$M(k) = f(0, k) = 1 + \int_0^\infty A(0, t)e^{ikt}\,dt, \tag{6.4}$$

but $|A(0, t)|$ is integrable because of the inequality (4.7).

From (6.1) and (6.2) and by using Wiener's theorem on the Fourier transform of absolutely integrable functions, we may deduce the following lemmas:

Lemma 6.2. *$W(k)$ possesses the following properties:*

(1) *$W(k)$ is a positive even function:*

$$W(k) > 0, \qquad W(-k) = W(k), \quad (-\infty < k < \infty); \tag{6.5}$$

(2) *$W(k) - 1$ has an absolutely integrable Fourier transform:*

$$W(k) = 1 + \int_{-\infty}^\infty H(t)e^{ikt}\,dt = 1 + 2\int_0^\infty H(t)\cos kt\,dt. \tag{6.6}$$

Lemma 6.3. *The function $S(k)$ possesses the following properties:*

(1) $|S(k)| = S(0) = S(\infty) = 1$,

$$S(-k) = S(k) = \overline{S(k)}^{-1}; \tag{6.7}$$

(2) *$S(k) - 1$ has an absolutely integrable Fourier transform:*

$$S(k) = 1 + \int_{-\infty}^\infty F(t)e^{-ikt}\,dt; \tag{6.8}$$

(3) $$\arg S(k)\,|_{-\infty}^{\infty} = -4i\pi m, \qquad m \geq 0, \tag{6.9}$$

where m is the number of discrete eigenvalues.

The last property is a consequence of the theorem for the number of zeros of an analytic function if we observe that $\arg S(k) = -2 \arg M(k)$. The properties of $W(k)$ and $S(k)$ enumerated in these lemmas are characteristic in the sense that, when they are fulfilled, there exists a unique function $M(s)$ which is analytic and bounded in the upper half-plane, and behaves asymptotically like $M(s) = 1 + o(1)$ for large $|s|$. Furthermore, $M(s)$ has a finite number of simple zeros $s_n = i\kappa_n$ $(n = 1, \cdots, m)$, and on the real axis, (6.1) and (6.2) are satisfied. In other words, there exists a function possessing the properties of the function $M(s)$ associated with some operator of type L having m discrete eigenvalues.

Let us first show that $M(s)$ is unique. Suppose there exists two functions $M_1(s)$ and $M_2(s)$, analytic and bounded in the upper half-plane $\tau > 0$, each having a finite number of zeros there at $s_n = i\kappa_n$ and such that, on the real axis,

$$S(k) = M_1(-k)/M_1(k) = M_2(-k)/M_2(k), \qquad (6.10)$$

where $S(k)$ is a given function satisfying the conditions of Lemma 6.3. Then $M_1(s)/M_2(s)$ is analytic and bounded in the upper half-plane and real on the real axis, so that it has a bounded analytic continuation into the lower half-plane. By Liouville's theorem, it follows that $M_1(s)/M_2(s) = C$. Thus, from the asymptotic behavior of M_1 and M_2 as $|s| \to \infty$, we find that $C = 1$, i.e., $M_1 = M_2$. By an analogous argument, we may prove that the function $M(s)$ satisfying (6.1) is unique [for a given $W(k)$]. It is necessary to consider $\ln (M_1/M_2)$.

We now complete the solution to our stated problem. We begin by reconstructing $M(k)$ from $S(k)$, and we consider first the case when $m = 0$ in (6.9). If we normalize the phase $\eta(k) = (i/2) \ln S(k)$ so that $\eta(0) = 0$, then $\eta(\infty) = 0$ and

$$\eta(k) = -\int_0^\infty \gamma(t) \sin kt \, dt, \quad \int_0^\infty |\gamma(t)| \, dt < \infty \qquad (6.11)$$

by the Wiener-Levi theorem. The function

$$M(k) = \exp \int_0^\infty \gamma(t) e^{ikt} \, dt \qquad (6.12)$$

is the solution of our problem. Suppose now that $m \neq 0$; the function

$$\tilde{S}(k) = S(k) \prod_{n=1}^{m} \left(\frac{k - i\kappa_n}{k + i\kappa_n} \right)^2 \qquad (6.13)$$

possesses the same properties as $S(k)$ with the exception that $\tilde{m} = 0$. Therefore, the relation

$$S(k) = \tilde{M}(-k)/\tilde{M}(k) \qquad (6.14)$$

holds where $\tilde{M}(s)$ has no zeros in the upper half-plane. The solution of our problem will then be the function

$$M(k) = \tilde{M}(k) \prod_{n=1}^{m} \frac{k - i\kappa_n}{k + i\kappa_n}. \qquad (6.15)$$

Consider now the determination of $M(k)$ for a given $W(k)$. By the Wiener-Levi theorem, the function $\rho(k) = \ln W(k)$ can be represented as

$$\rho(k) = -2 \int_0^\infty \gamma(t) \cos kt \, dt. \qquad (6.16)$$

The function

$$\tilde{M}(s) = \exp \int_0^\infty \gamma(t) e^{ist} \, dt \qquad (6.17)$$

is analytic in the upper half-plane, has no zeros there, and possesses the proper asymptotic behavior for large $|s|$. The solution of our problem will be the function

$$M(k) = \tilde{M}(k) \prod_{n=1}^{m} \frac{k - i\kappa_n}{k + i\kappa_n}. \qquad (6.18)$$

In the following, the functions $M(k)$, $W(k)$, and $S(k)$, related to some operator L, will be called the M, W, and S functions of this operator. Any of these functions characterize the spectrum of the corresponding operator L, with $M(k)$ giving the most complete characterization.

The following statements are a consequence of the above discussion.

(1) If L has no discrete spectrum then its S function is uniquely determined by its W function according to (6.16), (6.17), and (6.14).

(2) If two operators L_1 and L_2 have the same W function, L_1 has no discrete spectrum, but L_2 has discrete eigenvalues at $\lambda_n = -\kappa_n^2$ $(n = 1, \cdots, m)$, then their M and S functions are related by

$$M_1(k) = M_2(k) \prod_{n=1}^{m} \frac{k + i\kappa_n}{k - i\kappa_n},$$

$$S_1(k) = S_2(k) \prod_{n=1}^{m} \left(\frac{k - i\kappa_n}{k + i\kappa_n} \right)^2. \qquad (6.19)$$

These statements will be used in Secs. 8, 11, and 12.

7. THE TRANSFORMATION OPERATOR OF $A(x, y)$

In Sec. 4, besides U_B, we introduced an operator V_B with a kernel in the x representation determined by (4.10). In contrast to U_B, the operator V_B is not a transformation operator in the sense of Sec. 5. In fact, its kernel can not be represented as the Fourier sine transform of a solution of (1.1) satisfying a zero boundary condition. The present section is devoted to a clarification of the relationship between U_B and V_B. We shall assume that there is no discrete spectrum. This allows one to use the concise operator notation which was introduced in the preceding sections.

First consider the operator $\tilde{U}_B = U_B W$ which is the transformation operator related to the solution

$$\tilde{\varphi}(x, k) = \varphi(x, k) W(k) = \frac{1}{2ik} \left[\frac{f(x, k)}{M(k)} - \frac{f(x, -k)}{M(-k)} \right]. \qquad (7.1)$$

The kernel of the operator $\tilde{K} = \tilde{U}_B - I$ in the x representation is obtained by taking the Fourier transform of $\tilde{\varphi}(x, k) - k^{-1} \sin kx$:

$$\tilde{K}(x, y) = \frac{2}{\pi}\int_0^\infty \left(\tilde{\varphi}(x, k) - \frac{\sin kx}{k}\right)\frac{\sin ky}{k}\, k^2\, dk$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{f(x, k)}{M(k)} - e^{ikx}\right)e^{-iky}\, dk. \qquad (7.2)$$

By virtue of the analyticity and boundedness of $f(x, s)e^{-isx}/M(s)$ in the upper half-plane, $\tilde{K}(x, y) = 0$ for $x > y$. Therefore, the operator $\tilde{U}_B$ is given in the x representation by

$$\tilde{U}_B f(x) = f(x) + \int_x^\infty \tilde{K}(x, y)f(y)\, dy. \qquad (7.3)$$

In terms of $\tilde{U}_B$, the completeness and orthogonality relation

$$U_B W U_B^* = I \qquad (7.4)$$

becomes

$$\tilde{U}_B \tilde{W} \tilde{U}_B^* = I, \qquad \tilde{W} = W^{-1}, \qquad (7.5)$$

or

$$(\tilde{U}_B^*)^{-1} W (\tilde{U}_B)^{-1} = I. \qquad (7.6)$$

We note that $(\tilde{U}_B^*)^{-1}$ is a Volterra operator such as U_B, i.e., the integration goes from 0 to x. In Sec. 9, it will be shown that this Volterra operator is uniquely determined by (7.6). Hence, by comparing (7.4) and (7.6), we may conclude that

$$(\tilde{U}_B^*)^{-1} = U_B. \qquad (7.7)$$

This establishes the relationship between the two operators $\tilde{U}_B$ and U_B. On the other hand, by finding the inverse Fourier transform of

$$h(x, k) = \frac{f(x, k)}{M(k)} = e^{ikx} + \int_x^\infty \tilde{K}(x, y)e^{iky}\, dy, \qquad (7.8)$$

we can easily relate $\tilde{U}_B$ and V_B. Let $\Pi(t)$ denote the function

$$\Pi(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{1}{M(k)} - 1\right)e^{-ikt}\, dk. \qquad (7.9)$$

Since $1/M(s)$ is analytic in the upper half-plane (there is no discrete spectrum),

$$\Pi(t) = 0, \qquad t < 0. \qquad (7.10)$$

Recalling that

$$f(x, k) = e^{ikx} + \int_x^\infty A(x, y)e^{iky}\, dy, \qquad (7.11)$$

and using the convolution theorem, we find from (7.8) that

$$A(x, y) + \Pi(y - x) + \int_x^y A(x, t)\Pi(y - t)\, dt = \tilde{K}(x, y). \qquad (7.12)$$

This is the desired relation. It will be convenient to write this equation in operator form. With this in mind, we associate with $\Pi(t)$ an operator Q which in the coordinate representation is given by

$$Qf(x) = (I + \Pi)f(x) \equiv f(x) + \int_x^\infty \Pi(y - x)f(y)\, dy. \qquad (7.13)$$

By virtue of the boundedness of $1/M(s)$, it is not difficult to show that $Q = I + \Pi$ is a bounded operator in our Hilbert space. By means of known theorems on Volterra integral equations with difference-type kernels, it follows then that Q has an inverse

$$P = I + \Gamma = Q^{-1} \qquad (7.14)$$

whose structure in the x representation is similar to Q:

$$Pf(x) = (I + \Gamma)f(x) \equiv f(x) + \int_x^\infty \Gamma(y - x)f(y)\, dy. \qquad (7.15)$$

The function $\Gamma(t)$, i.e.,

$$\Gamma(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}(M(k) - 1)e^{-ikt}\, dk \qquad (7.16)$$

was introduced in the previous section [see (6.3)]. In terms of the operator Q, Eq. (7.12) becomes

$$\tilde{U}_B = V_B Q. \qquad (7.17)$$

The completeness and orthogonality of the eigenfunctions can now be written by using the operator V_B. The substitution of (7.17) in (7.5) yields

$$V_B Q W^{-1} Q^* V_B^* = I. \qquad (7.18)$$

Let us clarify the structure of the operator $QW^{-1}Q^*$. For this, the x representation is most convenient. In this representation, the operator $W^{-1} = \tilde{W}$ has the form $\tilde{W} = I + \tilde{\Omega}$ where $\tilde{\Omega}$ is an integral operator with the kernel

$$\tilde{\Omega}(x, y) = \frac{2}{\pi}\int_0^\infty \frac{\sin kx}{k}\left(\frac{1}{W(k)} - 1\right)$$

$$\times \frac{\sin ky}{k}\, k^2\, dk = \tilde{H}(x - y) - \tilde{H}(x + y), \qquad (7.19)$$

where

$$\tilde{H}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{1}{W(k)} - 1\right)e^{-ikt}\, dk. \qquad (7.20)$$

Denote by H_1 the operator with kernel $\tilde{H}(x - y)$ and by H_2 the operator with kernel $-\tilde{H}(x + y)$.

Then, the identity

$$[1/W(k)][1/M(k)] = M(-k) \tag{7.21}$$

can be expressed as

$$(I + \Pi)(I + H_1) = I + \Gamma^*. \tag{7.22}$$

Hence,

$$\begin{aligned} QW^{-1}Q^* &= (I + \Pi)(I + H_1 + H_2)(I + \Pi^*) \\ &= (I + \Gamma^* + (I + \Pi)H_2)(I + \Pi^*) \\ &= I + (I + \Pi)H_2(I + \Pi\ ). \end{aligned} \tag{7.23}$$

One can easily verify that the second term on the right-hand side of (7.23) is an integral operator whose kernel depends only on a sum and can be constructed using the function

$$\tilde{F}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(S(k) - \frac{1}{M^2(k)}\right)e^{ikt}\,dk. \tag{7.24}$$

For $t > 0$, $\tilde{F}(t)$ coincides with the function $F(t)$ introduced in the preceding section. We now associate with $F(t)$ the operator

$$Ff(x) = \int_0^{\infty} F(x + y)f(y)\,dy. \tag{7.25}$$

We have thus shown that the completeness and orthogonality relation for the eigenfunctions can be written in terms of V_B in the following way:

$$V_B(I - F)V_B^* = I. \tag{7.26}$$

To conclude this section, we point out the significance of the various operators in Hilbert space which have been applied. By the uniform boundedness of the functions $M(k)$, $1/M(k)$, $W(k)$, $1/W(k)$, and $S(k)$, the operators M, W, S, W^{-1}, M^{-1}, Q, P, and $I - F$ are bounded in our Hilbert space. Every other operator used, namely, U_B, $\tilde{U}_B$, and V_B, can be obtained from the unitary operator $U^{(+)}$ or $U^{(+)*}$ by multiplying by one of the above operators. Consequently, each of these operators is a bounded operator in our Hilbert space.

8. INTEGRAL EQUATIONS FOR THE KERNELS $K(x, y)$ AND $A(x, y)$

In this section, we shall show how the functions $W(k)$ and $S(k)$ and the kernels $K(x, y)$ and $A(x, y)$ are related. The completeness and orthogonality relations for the eigenfunctions expressed in terms of U_B and V_B are such expressions. However, if we write them out, for example, in the x representation, then the kernels $K(x, y)$ or $A(x, y)$ will enter nonlinearly. This is found to be unsuitable for solving the inverse problem. Nevertheless, the fact that U_B and V_B are Volterra operators in the x representation allows one to easily obtain expressions relating $W(k)$ and $S(k)$ and the kernels $K(x, y)$ and $A(x, y)$ in which the latter enter linearly.

For simplicity, we first assume that there is no discrete spectrum. Expressing the equality

$$U_B W U_B^* = I \tag{8.1}$$

in the form

$$U_B W = \tilde{U}_B, \qquad \tilde{U}_B = (U_B^*)^{-1} \tag{8.2}$$

and then writing out (8.2) in the x representation, we obtain

$$K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\,dt = \tilde{K}(x, y). \tag{8.3}$$

Here

$$\Omega(x, y) = \frac{2}{\pi}\int_0^{\infty}\frac{\sin kx}{k}\,[W(k) - 1]\,\frac{\sin ky}{k}\,k^2\,dk. \tag{8.4}$$

Since $\tilde{K}(x, y) = 0$ for $x > y$ [see (7.2)], it finally follows that

$$K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\,dt = 0, \qquad x > y. \tag{8.5}$$

In an analogous way, the relation

$$V_B(I - F)V_B^* = I \tag{8.6}$$

gives

$$A(x, y) = F(x + y) + \int_x^{\infty} A(x, t)F(t + y)\,dt, \qquad x < y, \tag{8.7}$$

$$F(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}(S(k) - 1)e^{ikt}\,dk. \tag{8.8}$$

In case there is a discrete spectrum, similar equations can be obtained by starting directly from the representation (4.3) for $\varphi(x, k)$ and the completeness and orthogonality relation in the form (2.6). An equation for the transformation operator which relates the solutions $\varphi(x, k)$ of two different equations of the form (1.1) will now be derived. We begin with the following relations [cf. (2.6)]:

$$\varphi_2(x, k) = \varphi_1(x, k) + \int_0^x K(x, t)\varphi_1(t, k)\,dt, \tag{8.9}$$

$$\varphi_1(y, k) = \varphi_2(y, k) + \int_0^y \tilde{K}(t, y)\varphi_2(t, k)\,dt, \tag{8.10}$$

$$\sum_{n_i=1}^{m_i} C_{n_i}\varphi_{n_i}(x)\varphi_{n_i}(y) + \frac{2}{\pi}\int_0^\infty \varphi_i(x, k)W_i(k)\varphi_i(y, k)k^2\,dk = \delta(x-y) \qquad (i = 1, 2). \tag{8.11}$$

If both sides of (8.10) are multiplied by $\phi_2(x, k)\cdot W_2(k)k^2$ and integrated with respect to k, and then (8.11) for $i = 2$ is used, there results

$$\frac{2}{\pi}\int_0^\infty \varphi_2(x, k)W_2(k)\varphi_1(y, k)k^2\,dk + \sum_{n_2=1}^{m_2} C_{n_2}\varphi_1(y, i\kappa_{n_2})\varphi_{n_2}(x) = \delta(x-y) + \int_0^y \tilde{K}(t, y)\,\delta(x-t)\,dt = \delta(x-y), \qquad x > y. \tag{8.12}$$

Analogous operations on (8.9) with the use of (8.12) then yield

$$\delta(x-y) = \frac{2}{\pi}\int_0^\infty \varphi_1(x, k)W_2(k)\varphi_1(y, k)k^2\,dk + \sum_{n_2=1}^{m_2} C_{n_2}\varphi_1(x, i\kappa_{n_2})\varphi_1(y, i\kappa_{n_2}) + \int_0^x K(x, t)\left[\frac{2}{\pi}\int_0^\infty \varphi_1(t, k)W_2(k)\varphi_1(y, k)k^2\,dk + \sum_{n_2=1}^{m_2} C_{n_2}\varphi_1(t, i\kappa_{n_2})\varphi_1(y, i\kappa_{n_2})\right]dt, \qquad x > y. \tag{8.13}$$

Subtracting (8.11) for $i = 1$ from (8.13), we finally obtain, after simple computations,

$$K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\,dt = 0, \qquad x > y, \tag{8.14}$$

where

$$\Omega(x, y) = \frac{2}{\pi}\int_0^\infty \varphi_1(x, k)[W_2(k) - W_1(k)]\varphi_1(y, k)k^2\,dk + \sum_{n_2=1}^{m_2} C_{n_2}\varphi_1(x, i\kappa_{n_2})\varphi_1(y, i\kappa_{n_2}) - \sum_{n_1=1}^{m_1} C_{n_1}\varphi_{n_1}(x)\varphi_{n_1}(y). \tag{8.15}$$

Since the generalization of (8.7) will not be required later on, its derivation is omitted. Equations (8.5) and (8.14) are called the Gel'fand-Levitan equations, and (8.7) is called the Marchenko equation.

These equations enable one to solve inverse problems, i.e., to reconstruct the operator L under different formulations. We first apply these equations in the solution of the following two problems.

(1) Given a function $W(k)$ having the properties enumerated in Lemma 6.2. To construct an operator L with no discrete spectrum for which $W(k)$ is its W function.

(2) Given an operator L_1 [$q_1(x) \not\equiv 0$] with no discrete spectrum such that $W_1(k)$ is its W function. To construct an operator L whose W function is $W_1(k)$ and which has discrete eigenvalues at prescribed points $\lambda_n = -\kappa_n^2$ ($n = 1, \cdots, m$).

The basic problem, i.e., the determination of L from its S function and its discrete energy levels, will be solvable if these two problems can be solved. Let there be given m distinct positive numbers κ_n ($n = 1, 2, \cdots, m$) and a function $S(k)$ possessing the properties enumerated in Lemma 6.3. By the procedure of Sec. 6, $W(k)$ can be constructed uniquely from this data. If in conjunction with problem 1, we now construct an operator $\tilde{L}$ without a discrete spectrum for which this $W(k)$ is its W function then, by the statements at the end of Sec. 6, the S function of this operator will be

$$\tilde{S}(k) = S(k)\prod_{n=1}^{m}\left(\frac{k - i\kappa_n}{k + i\kappa_n}\right)^2. \tag{8.16}$$

If in accordance with problem 2, we now start with the operator $\tilde{L}_1$ and construct an operator L which has $W(k)$ as its W function and the m points $\lambda_n = -\kappa_n^2$ as its discrete eigenvalues, then L will have the initially-given function $S(k)$ as its S function, and the basic problem will therefore be solved.

9. EXISTENCE OF A SOLUTION OF THE GEL'FAND-LEVITAN EQUATION. SOLUTION OF THE FIRST PROBLEM

Let us proceed to solve the two problems formulated in the previous section. To this end, we shall make use of the Gel'fand-Levitan equations (8.5), (8.4) and (8.14), (8.15), and we therefore first show that they have solutions.

We go directly to the general equation (8.14). Let the operator L_1 be given. That is, its eigenfunctions $\varphi_1(x, k)$, its W function $W_1(k)$, its discrete eigenvalues $\lambda_{n_1} = -\kappa_{n_1}^2$ and corresponding normalizing factors C_{n_1} are prescribed. Also, let the function $W(k)$ having the properties enumerated in Lemma 6.2 and the arbitrary positive numbers κ_n and C_n be prescribed. Assume that the κ_n are distinct. From this data, we construct the function $\Omega(x, y)$ by means of (8.15). By virtue of our given conditions, this function will be absolutely inte-

grable with respect to x or y in any finite interval. Equation (8.14) for $K(x, y)$ is an equation with respect to the argument y, the kernel and free term depending on x as a parameter. For fixed x, this equation is a Fredholm equation. Therefore, to show that a unique solution exists, it suffices to prove that the homogeneous equation has only a trivial solution.

Suppose that for fixed x_0, the equation

$$h_0(y) + \int_0^{x_0} h_0(t)\Omega(t, y)\, dt = 0 \tag{9.1}$$

has a solution. Denote

$$h(y) = \begin{cases} h_0(y) & \text{for } y \leq x_0, \\ 0 & \text{for } y > x_0. \end{cases} \tag{9.2}$$

Multiplying (9.1) by $h(y)$ and integrating with respect to y, we obtain

$$\int_0^\infty h^2(y)\, dy + \int_0^\infty \int_0^\infty h(t)\Omega(t, y)h(y)\, dt\, dy = 0. \tag{9.3}$$

The substitution of the expression (8.15) for $\Omega(x, y)$ in this yields

$$\begin{aligned} &\int_0^\infty h^2(y)\, dy + \frac{2}{\pi}\int_0^\infty \left[\int_0^\infty h(y)\varphi_1(y, k)\, dy\right]^2 \\ &\quad \times [W_2(k) - W_1(k)]k^2\, dk \\ &\quad + \sum_{n=1}^{m} C_n\left[\int_0^\infty h(y)\varphi_1(y, i\kappa_n)\, dy\right]^2 \\ &\quad - \sum_{n_1=1}^{m_1} C_{n_1}\left[\int_0^\infty h(y)\varphi_{n_1}(y)\, dy\right]^2 = 0. \end{aligned} \tag{9.4}$$

By means of Parseval's equality for the system of functions $\varphi_1(x, k)$ this may be simplified to

$$\begin{aligned} &\frac{2}{\pi}\int_0^\infty \left[\int_0^\infty h(y)\varphi_1(y, k)\, dy\right]^2 W_2(k)k^2\, dk \\ &\quad + \sum_{n=1}^{m} C_n\left[\int_0^\infty h(y)\varphi_1(y, i\kappa_n)\, dy\right]^2 = 0. \end{aligned} \tag{9.5}$$

Since $W_2(k)$ is positive, this implies that $h(y)$ is orthogonal to the subspace corresponding to the continuous spectrum of L. Consequently, $W_2(k)$ is a linear combination of eigenfunctions of the discrete spectrum. But this is impossible since $h(y)$ vanishes identically for $y > x_0$, and hence $h(y) \equiv 0$.

The remainder of this section and the two succeeding sections will be devoted to solving the first problem. In so doing, we must consider the equation

$$K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\, dt = 0, \qquad x > y, \tag{9.6}$$

$$\Omega(x, y) = \frac{2}{\pi}\int_0^\infty \frac{\sin kx}{k}\,(W(k) - 1)\,\frac{\sin ky}{k}\,k^2\, dk, \tag{9.7}$$

which was obtained from the condition

$$U_B W U_B^* = I \tag{9.8}$$

for the operator $U_B = I + K$. Conversely, we shall show that the operator $U_B = I + K$, defined in terms of the solution of (9.6), has the property (9.8), where the function $W(k)$ only has to satisfy the conditions enumerated in Lemma 6.2.

We note that the solution of (9.6) also determines a kernel $\tilde{K}(x, y)$ which is different from zero only for $x < y$:

$$\tilde{K}(x, y) = \begin{cases} K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\, dt, \\ \qquad\qquad x < y, \\ 0, \qquad\qquad x > y. \end{cases} \tag{9.9}$$

With this kernel, we associate the operator $\tilde{K}$. Let $\tilde{U}_B = I + \tilde{K}$. In terms of U_B and $\tilde{U}_B$, relation (9.9) becomes

$$U_B W = \tilde{U}_B, \tag{9.10}$$

and to prove (9.8), we must now show that

$$U_B = (\tilde{U}_B^*)^{-1}. \tag{9.11}$$

Since $W(k)$ is real, W is self-adjoint. From (9.10), it follows that $\tilde{U}_B U_B^* = U_B W U_B^*$ so that $\tilde{U}_B U_B^*$ is also self-adjoint. On the other hand, since $\tilde{U}_B$ and U_B^* are Volterra operators, $\tilde{U}_B U_B^*$ is also a Volterra operator and this property together with the self-adjointness implies that $\tilde{U}_B U_B^* = I$. This is what we had to show.

The above reasoning is of a rather formal character since no estimates for $K(x, y)$ and $\tilde{K}(x, y)$ were given that would have explained the meaning of U_B and $\tilde{U}_B$ as operators in Hilbert space. However, the relation (9.8), when written out in the x representation, only involves integrals over finite intervals of integration (whose existence it is therefore not necessary to prove), and this relation may be proved starting directly from (9.6). Inasmuch as this relation is proven, it is possible to attach meaning to the operator U_B. In fact, the function $M(k)$ constructed from $W(k)$ by the procedure of Sec. 6, is a bounded function and a bounded operator can be associated with it, namely, an operator which

multiplies by $M(k)$ in the momentum representation. Since $M(k) \neq 0$, the operator M^{-1} is also bounded. From (9.8), we find that $U^{(+)} = U_B M^{-1}$ is unitary and from this follows the boundedness of U_B.

With the operator thus obtained, we define an operator L by

$$L = U_B L_0 U_B^{-1}, \tag{9.12}$$

where L_0 is the operator which multiplies by k^2 in the k representation, which was introduced in Secs. 3 and 5. Now $L = U_B L_0 W U_B^*$ by virtue of (9.8), and hence, L is self-adjoint because W and L_0 commute. On the basis of Theorem 5.2, we can say that L is a differential operator in the x representation associated with an equation of the form (1.1) with a potential given by

$$q(x) = 2\, dK(x, x)/dx. \tag{9.13}$$

Equation (9.8) shows that the given function $W(k)$ is the W function for L. And so, the first problem of Sec. 8 is solved in the sense that an operator L has been shown to exist. The properties of the potential $q(x)$ obtained in the solution of this problem will be investigated in the following section.

In conclusion, we note that our considerations imply that (9.8) determines the Volterra operator U_B uniquely. This fact was previously used in Sec. 7.

10. MARCHENKO'S EQUATION. THE PROPERTIES OF THE POTENTIAL

To study the properties of $q(x)$, we find it convenient to use Marchenko's equation

$$A(x, y) = F(x + y) + \int_x^\infty A(x, t)F(t + y)\, dt, \qquad x < y, \tag{10.1}$$

in which

$$F(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} [S(k) - 1] \exp(ikt)\, dk. \tag{10.2}$$

The existence of a solution of (10.1) will not be proved. Instead, we show that (10.1) is equivalent to the Gel'fand-Levitan equation (8.5) provided, of course, that the corresponding functions $W(k)$ and $S(k)$ are related by the formulas of Sec. 6. In the preceding section, it was shown that the Gel'fand-Levitan equation (8.5) and the relation $U_B W U_B^* = I$ for the operator $U_B = I + K$ are equivalent. By repeating the reasoning of Secs. 7 and 8, we find that $V_B = \tilde{U}_B Q^{-1}$ is an operator which can be constructed using the solution $A(x, y)$ of (10.1). Therefore (10.1) has a solution for any $x \geq 0$. Conversely, it is not difficult to show that if the operator V_B is formed with respect to a solution of (10.1), then $U_B = (Q^* V_B^*)^{-1}$ is the operator formed by using the solution of the Gel'fand-Levitan equation (8.5). This implies the uniqueness of a solution of (10.1).

The potential $q(x) = 2\, dK(x, x)/dx$ can be expressed very simply in terms of $A(x, y)$. In fact, from (7.12) it follows that $A(x, x) = \tilde{K}(x, x) - \Pi(0)$ and $dA(x, x)/dx = d\tilde{K}(x, x)/dx$. If (7.7) is written out in terms of $K(x, y)$ and $\tilde{K}(x, y)$, we obtain

$$\tilde{K}(y, x) + K(x, y) + \int_y^x \tilde{K}(t, x)K(t, y)\, dt = 0, \tag{10.3}$$

from which it follows that

$$dK(x, x)/dx = -d\tilde{K}(x, x)/dx.$$

Finally,

$$q(x) = 2\, dK(x, x)/dx = -2\, dA(x, x)/dx. \tag{10.4}$$

The solution of (10.1) will now be investigated. It turns out that $q(x)$ behaves in many respects like the derivative of $F(t)$ for $t > 0$. We shall derive some estimates, and we first consider how $F'(t)$ behaves in relation to $q(x)$. It is convenient to introduce the functions

$$\sigma(x) = \int_x^\infty |q(t)|\, dt, \quad \sigma_1(x) = \int_x^\infty t\, |q(t)|\, dt. \tag{10.5}$$

The estimates given in Sec. 4 for $A(x, y)$ and $\partial A(x, y)/\partial x$ can now be expressed as

$$|A(x, y)| \leq K\sigma[\tfrac{1}{2}(x + y)] \tag{10.6}$$

$$|\partial A(x, y)/\partial x + \tfrac{1}{4}q[\tfrac{1}{2}(x + y)]| \leq K\sigma[\tfrac{1}{2}(x + y)]\sigma(x). \tag{10.7}$$

In (10.1), we set $x = y$. Then

$$A(x, x) = F(2x) + \int_x^\infty A(x, t)F(t + x)\, dt \tag{10.8}$$

or

$$F(2x) = A(x, x) - 2\int_x^\infty A(x, 2t - x)F(2t)\, dt. \tag{10.9}$$

The last equation may be solved by the method of successive approximations and the following estimate for its solution may be derived:

$$|F(2x)| \leq K\sigma(x). \tag{10.10}$$

Differentiation of (10.9) with respect to x and the use of the inequalities (10.7) and (10.10) then yield

$$|F'(2x) + \tfrac{1}{4}q(x)| \leq K\sigma^2(x). \tag{10.11}$$

Conversely, we now consider the question, how $q(x)$ relates to $F'(t)$, for which it is convenient to transform (10.1) into

$$A(x, x + y) = F(2x + y) + \int_0^\infty A(x, x + t)F(2x + t + y)\, dt. \quad (10.12)$$

Let F_x denote the operator

$$F_x g(y) = \int_0^\infty g(t)F(2x + t + y)\, dt. \quad (10.13)$$

Because (10.1) has a unique solution for any x and since the norm of F_x is small for large x, the norm of $(I - F_x)^{-1}$ is uniformly bounded in $\mathfrak{L}_1(0, \infty)$. Hence,

$$\int_0^\infty |A(x, x + y)|\, dy = \int_x^\infty |A(x, y)|\, dy \leq K \int_{2x}^\infty |F(t)|\, dt. \quad (10.14)$$

Introduce now the notation

$$\tau(x) = \int_x^\infty |F'(t)|\, dt, \qquad \tau_1(x) = \int_x^\infty t\, |F'(t)|\, dt. \quad (10.15)$$

Then,

$$|F(x)| \leq \int_x^\infty |F'(t)|\, dt = \tau(x). \quad (10.16)$$

From (10.1) and the inequality (10.14), we obtain the uniform estimate

$$|A(x, y)| \leq K\tau(x + y). \quad (10.17)$$

We next consider the differentiability of $A(x, x)$, and we set

$$B(x, y) = A(x, x + y). \quad (10.18)$$

The difference quotient

$$\Delta_x B(x, y)/h = [B(x + h, y) - B(x, y)]/h \quad (10.19)$$

satisfies an equation of the same type as does $B(x, y)$:

$$\frac{\Delta_x B(x, y)}{h} = \frac{\Delta_x F(2x + y)}{h} + \int_0^\infty B(x, t)\, \frac{\Delta_x F(2x + t + y)}{h}\, dt + \int_0^\infty \frac{\Delta_x B(x, t)}{h}\, F(2x + 2h + t + y)\, dt. \quad (10.20)$$

The free term

$$\frac{\Delta_x F(2x + y)}{h} + \int_0^\infty B(x, y)\, \frac{\Delta_x F(2x + t + y)}{h}\, dt \quad (10.21)$$

can be estimated, uniformly in h, because of the differentiability of $F(t)$, whence follows the differentiability of $B(x, y)$. Moreover, just as in the above way, we obtain an estimate for $\partial B(x, y)/\partial x$:

$$\int_0^\infty \left|\frac{\partial B}{\partial x}(x, y)\right| dy \leq K\tau(2x). \quad (10.22)$$

This, in turn, leads to the estimate

$$|dA(x, x)/dx - 2F(2x)| \leq K\tau^2(2x) \quad (10.23)$$

or

$$|F'(2x) + \tfrac{1}{4}q(x)| \leq K\tau^2(2x). \quad (10.24)$$

Thus the inequalities (10.11) and (10.24) explicitly show the analogous behavior of $q(x)$ and $F'(2x)$. In particular, if

$$\int_0^\infty x\, |q(x)|\, dx < \infty \quad (10.25)$$

then

$$\int_0^\infty x\, |F'(2x)|\, dx < \infty, \quad (10.26)$$

and conversely. These inequalities may also be used to establish necessary and sufficient conditions on the S function assuring that the corresponding potential decreases like x^{-n} or exponentially, or vanishes identically for $x > A$, etc. A precise formulation of these conditions will not be given here because of the lack of space.

11. KREIN'S EQUATION. ASYMPTOTIC BEHAVIOR OF $\varphi(k, x)$

The eigenfunctions $\varphi(x, k)$ of the operator L are formed according to the formula

$$\varphi(x, k) = \frac{\sin kx}{k} + \int_0^x K(x, y)\, \frac{\sin ky}{k}\, dy. \quad (11.1)$$

These functions behave asymptotically like [cf. (1.21)]

$$\varphi(x, k) \approx [A(k)/k] \times \sin [kx - \eta(k)], \qquad x \to \infty, \quad (11.2)$$

in which $A(k)$ and $\eta(k)$ are, respectively, the modulus and argument of the M function of L which is uniquely determined by $W(k)$ by the relation

$$W(k) = 1/[M(k)M(-k)] \quad (11.3)$$

and the condition of analyticity (see Sec. 6).

It is not easy to deduce the asymptotic expression (11.2) directly from (11.1). Another representation for $\varphi(x, k)$ will therefore be obtained from which (11.2) can be deduced without difficulty. Of course, this representation not only serves to prove (11.2), but the procedure used to obtain it is interesting *per se*, in that it reveals more completely the structure of the kernel $A(x, y)$ of the transformation operator.

The starting point is the Gel'fand-Levitan equation

$$K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\, dt = 0, \qquad y < x, \tag{11.4}$$

in which

$$\Omega(x, y) = \frac{2}{\pi}\int_0^\infty \sin kx[W(k) - 1] \sin ky\, dk. \tag{11.5}$$

We can obviously write

$$\Omega(x, y) = H(x - y) - H(x + y), \tag{11.6}$$

where the function

$$H(t) = \frac{1}{\pi}\int_0^\infty [W(k) - 1] \cos kt\, dk \tag{11.7}$$

is the one previously introduced in Sec. 6 [see (6.6)]. If a solution $K(x, y)$ is sought in the form

$$K(x, y) = \Gamma_{2x}(x - y) - \Gamma_{2x}(x + y), \tag{11.8}$$

then one obtains for $\Gamma_{2x}(t)$, the equation

$$\Gamma_{2x}(t) + H(t) + \int_0^{2x} \Gamma_{2x}(s)H(s - t)\, ds = 0, \tag{11.9}$$

which is equivalent to (11.4). This is an equation for $\Gamma_{2x}(t)$ in the argument t, x playing the role of a parameter. This fact underscores the unsymmetric dependence of $\Gamma_{2x}(t)$ on its arguments. We shall call (11.9) Krein's equation. Knowing its solution, we can easily find the kernel $K(x, y)$, and together with it, the potential $q(x)$ and the solution $\varphi(x, k)$. However, these functions can be expressed directly in terms of $\Gamma_{2x}(t)$, as follows.

If we denote by $G_a(x, t)$ the resolvent of the kernel $H(x - t)$ on the interval $(0, a)$:

$$G_a(x, t) + H(x - t) + \int_0^a G_a(x, s)H(s - t)\, ds = 0, \tag{11.10}$$

then

$$\Gamma_{2x}(t) = G_{2x}(0, t). \tag{11.11}$$

We now note some properties of $G_a(x, t)$. Differentiation of (11.10) with respect to a shows that $G_a(x, t)$ satisfies

$$\partial G_a(x, t)/\partial a = G_a(x, a)G_a(a, t). \tag{11.12}$$

Also,

$$G_a(t, s) = G_a(a - t, a - s). \tag{11.13}$$

We next express $q(x) = 2\, dK(x, x)/dx$ in terms of $\Gamma_{2x}(t) = G_{2x}(0, t)$:

$$q(x) = 2\, dG_{2x}(0, 0)/dx - 2\, dG_{2x}(0, 2x)/dx. \tag{11.14}$$

If the notation

$$A(x) = 2G_{2x}(0, 2x) = 2\Gamma_{2x}(2x) \tag{11.15}$$

is introduced, then by virtue of (11.12) and (11.13)

$$q(x) = -dA(x)/dx + A^2(x). \tag{11.16}$$

This last formula enables us to reduce our second-order differential equation containing $q(x)$ to a system of equations of the first order. Thus,

$$d^2/dx^2 - q(x) = [d/dx - A(x)][d/dx + A(x)] \tag{11.17}$$

and the equation

$$-y'' + q(x)y = k^2 y \tag{11.18}$$

is equivalent to the system

$$\left.\begin{aligned} dy/dx + Ay &= kz, \\ -dz/dx + Az &= ky. \end{aligned}\right\} \tag{11.19}$$

In certain cases, this system turns out to be more convenient than the original equation (11.18). Let us now express the solution $\varphi(x, k)$ in terms of $\Gamma_{2x}(t)$:

$$\begin{aligned}\varphi(x, k) &= \frac{\sin kx}{k} + \int_0^x \Gamma_{2x}(x - y)\frac{\sin ky}{k}\, dy \\ &\quad - \int_0^x \Gamma_{2x}(x + y)\frac{\sin ky}{k}\, dy \\ &= \frac{\sin kx}{k} + \int_0^{2x} \Gamma_{2x}(t)\frac{\sin k(x - t)}{k}\, dt \\ &= \frac{1}{k}\operatorname{Im}\left[e^{ikx}\left(1 + \int_0^{2x} \Gamma_{2x}(t)e^{-ikt}\, dt\right)\right].\end{aligned} \tag{11.20}$$

When $x \to \infty$, we find that

$$\varphi(x, k) \to \frac{1}{k}\operatorname{Im}\left[e^{ikx}\left(1 + \int_0^\infty \Gamma(t)e^{-ikt}\, dt\right)\right], \tag{11.21}$$

where $\Gamma(t) = \lim_{x\to\infty} \Gamma_{2x}(t)$ is the solution of the equation

$$\Gamma(t) + H(t) + \int_0^\infty \Gamma(s)H(t-s)\,ds = 0. \qquad (11.22)$$

That is, this equation is satisfied by the function

$$\Gamma(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} (M(k) - 1)e^{-ikt}\,dk, \qquad (11.23)$$

introduced in Sec. 6 [see (6.3)]. This is not difficult to show if one takes the Fourier transform of the identity (11.3) re-expressed in the form

$$(W(k) - 1)(M(k) - 1) + (M(k) - 1) + (W(k) - 1) = 1/M(-k) - 1, \qquad (11.24)$$

and takes into consideration that $1/M(-k)$ is analytic in the lower half-plane. Thus, from (11.21), it follows that

$$\varphi(x, k) \to (1/k)\ \mathrm{Im}\ \{M(-k)e^{-ikx}\} \qquad (11.25)$$

as $x \to \infty$ and this, in turn, yields the asymptotic behavior (11.2).

12. RELATIONSHIP OF THE OPERATORS TO THE DISCRETE SPECTRA

In line with our program, we have completed the solution of the first problem and in this section we solve the second problem. We must consider the Gel'fand-Levitan equation (8.14) for the case where the given operator L_1 has no discrete spectrum, i.e. all $C_{n_1} = 0$, and where the required operator has the discrete eigenvalues $\lambda_n = -\kappa_n^2$ $(n = 1, 2, \cdots, m)$ with corresponding normalizing factors C_n and the same W function as L_1. The equation in this case is given by

$$K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\,dt = 0, \qquad x > y, \qquad (12.1)$$

with

$$\Omega(x, y) = \sum_{n=1}^{m} C_n\varphi_1(x, i\kappa_n)\varphi_1(y, i\kappa_n). \qquad (12.2)$$

This is an equation with a degenerate kernel and is easily solved. For this, it is advantageous to use vector notation. Thus we write $\Omega(x, y)$ in the form

$$\Omega(x, y) = (\psi(x), \varphi(y)), \qquad (12.3)$$

where $\psi(x)$ and $\varphi(y)$ are vectors with the components $C_n\varphi_1(x, i\kappa_n)$ and $\varphi_1(y, i\kappa_n)$, respectively. We seek a solution of (12.1) in the form

$$K(x, y) = (\mathbf{a}(x), \varphi(y)), \qquad (12.4)$$

and the Gel'fand-Levitan equation becomes

$$(\mathbf{a}(x), \varphi(y_j)) + (\psi(x), \varphi(y)) + \left(\int_0^x R(t)\,dt\mathbf{a}(x), \varphi(y)\right) = 0. \qquad (12.5)$$

Here $R(t)$ is the tensor product of the vectors $\varphi(t)$ and $\psi(t)$, i.e., the matrix with elements

$$r_{ik}(t) = \varphi_i(t)\psi_k(t) \qquad (i, k = 1, \cdots, m). \qquad (12.6)$$

Consider the matrix

$$V(x) = I + \int_0^x R(t)\,dt. \qquad (12.7)$$

The general result on the existence of a solution of the Gel'fand-Levitan equation enables us to say that the matrix $V(x)$ has an inverse for all x. However, from its definition, one may easily verify that $V(x)$ is positive-definite.

By virtue of (12.4) and (12.5), we have

$$K(x, y) = -[V(x)^{-1}\psi(x), \varphi(y)], \qquad (12.8)$$

and, in particular,

$$K(x, x) = -[V(x)^{-1}\psi(x), \varphi(x)] = -\mathrm{Tr}\,[V(x)^{-1}R(x)] = -\mathrm{Tr}\left[V(x)^{-1}\frac{d}{dx}V(x)\right] = -\frac{d}{dx}\ln\det V(x), \qquad (12.9)$$

since

$$R(x) = dV(x)/dx. \qquad (12.10)$$

By an analysis of the general Gel'fand-Levitan equation (8.14) similar to that previously carried out for (8.5), it may be shown that in the x representation, the operator

$$L = U_B L_1 U_B^{-1}, \qquad (12.11)$$

defined in terms of the solution $K(x, y)$ of this equation, is a differential operator with a potential $q(x) = q_1(x) + \Delta q(x)$, where

$$\Delta q(x) = 2\,dK(x, x)/dx. \qquad (12.12)$$

Moreover, its eigenfunctions are determined by

$$\varphi(x, k) = \varphi_1(x, k) + \int_0^x K(x, y)\varphi_1(y, k)\,dy, \qquad (12.13)$$

its W function is the function $W(k)$, and the quantities $\lambda_n = -\kappa_n^2$ $(n = 1, \cdots, m)$ are the points of its discrete spectrum. Such an analysis will not be carried out, and the above statements for the problem in question will be proved by other simpler means. In Sec. 15, it will be shown that the function $\varphi(x, k)$ determined by (12.13) is a solution of (1.1)

with a potential $q(x) = q_1(x) + \Delta q(x)$, where $\Delta q(x)$ is given by (12.12). In this section, the properties of these functions will be examined.

By (12.8), (12.9), and (12.12), the following formulas for $\Delta q(x)$ and $\varphi(x, k)$ hold:

$$\Delta q(x) = -2(d^2/dx^2) \ln ||V(x)||,$$

$$||V(x)|| = \det V(x), \qquad (12.14)$$

$$\varphi(x, k) = \begin{Vmatrix} V(x) & \psi(x) \\ \beta(x, k) & \varphi_1(x, k) \end{Vmatrix} \Big/ ||V(x)||. \qquad (12.15)$$

The determinant in the numerator of (12.15) is that of the matrix obtained by bordering the matrix $V(x)$ with the vectors $\psi(x)$ and $\beta(x, k)$ and the function $\varphi_1(x, k)$, where

$$\beta(x, k) = \int_0^x \varphi(y)\varphi_1(y, k)\, dy. \qquad (12.16)$$

The M function of L can be found from the asymptotic expansion of the solution $\varphi(x, k)$. We next investigate this asymptotic behavior and also the properties of the potential increment $\Delta q(x)$ directly from (12.14) and (12.15), confining ourselves, for simplicity, to the case $m = 1$. We make use of the fact that $\varphi_1(x, i\alpha)$, $\alpha > 0$, behaves asymptotically like [see (1.7)]

$$\varphi_1(x, i\alpha) = Ne^{\alpha x}[1 + o(1)], \qquad (x \to \infty), \qquad (12.17)$$

and

$$\varphi_1(x, i\alpha) = x[1 + o(1)]x, \qquad (x \to 0). \qquad (12.18)$$

Express $\varphi(x, k)$ as the sum of two terms

$$\varphi(x, k) = (1/2ik)[h(x, k) - h(x, -k)], \qquad (12.19)$$

where

$$h(x, k) = M(-k) \exp(ikx) + o(1) \qquad (12.20)$$

as $x \to \infty$. Equation (12.15) then yields

$$h(x, k) = h_1(x, k) - \frac{C\varphi_1(x, i\kappa)}{1 + C\int_0^x [\varphi_1(t, i\kappa)]^2\, dt} \times \int_0^x \varphi_1(x, i\kappa)h_1(x, k)\, dx$$

$$= M_1(-k)\left[e^{ikx} - \frac{CNe^{\kappa x}}{C(N^2/2\kappa)e^{2\kappa x}} \frac{N}{\kappa + ik} e^{ikx+\kappa x}\right]$$

$$+ o(1) = M_1(-k)\frac{k + i\kappa}{k - i\kappa} e^{ikx} + o(1), \qquad (12.21)$$

so that

$$M(k) = M_1(k)(k - i\kappa)/(k + i\kappa). \qquad (12.22)$$

Hence, it follows that $\lambda = -\kappa^2$ is an eigenvalue of L.

Let us now consider $\Delta q(x)$. By virtue of its definition (12.7), $V(x)$ is twice differentiable even if the potential $q_1(x)$ for the given operator is a generalized function with δ-type singularities. Therefore, $\Delta q(x)$ is always an ordinary summable function. As $x \to 0$,

$$\Delta q(x) = -2\frac{d^2}{dx^2} \ln\left\{1 + C\int_0^x t^2[1 + o(1)]\, dt\right\} = -4Cx[1 + o(1)], \qquad (12.23)$$

and as $x \to \infty$,

$$\Delta q(x) = -2\frac{V''(x)V(x) - (V'(x))^2}{V^2(x)} = -(2/C)(2\kappa)^3 e^{-2\kappa x}[1 + o(1)]. \qquad (12.24)$$

If $m > 1$, asymptotic forms similar to (12.23) and (12.24) still hold for $\Delta q(x)$, in which $C = \sum_{n=1}^m C_n$ in (12.23) and $C = C_r$, $\kappa = \kappa_r$ in (12.24), κ_r being the smallest of the κ_n. At all events,

$$\int_0^\infty x\, |\Delta q(x)|\, dx < \infty. \qquad (12.25)$$

The solution of the second problem of Sec. 8, except for the one statement to be proved in Sec. 15, is thus complete. The solution is given by (12.14) and (12.15). In these formulas, $C_1, C_2, \cdots C_m$ may be any positive numbers, so that we have an m-parameter family of solutions. Formula (12.14) is the formula for the equivalent potentials given by Jost and Kohn.

This simultaneously completes the solution of the basic inverse problem. The results obtained in Secs. 9 to 12 are summarized in the following theorem.

Theorem 12.1. *Any function $S(k)$ with the properties*

(1) $|S(k)| = S(\infty) = S(0) = 1$,

(2) $S(-k) = \overline{S}(k) = S^{-1}(k)$,

(3) $S(k) = 1 + \int_{-\infty}^{\infty} F(t) \exp(-ikt)\, dt$, where $\int_{-\infty}^{\infty} |F(t)|\, dt < \infty$,

(4) $\arg S(k)\,|_{-\infty}^{\infty} = -4i\pi m, \qquad m \geq 0,$

is the S function of some operator having m negative eigenvalues and a continuous spectrum along the half-ray $(0, \infty)$. In the x representation, it is a differential operator of type (1.1) *with a potential that may be a generalized function such as the derivative of a locally summable function.*

In order for the condition $\int_0^\infty x\, |q(x)|\, dx < \infty$ to hold, it is necessary and sufficient that $\int_0^\infty t\, |F'(t)|\, dt < \infty$.

If $m > 0$, the potential is not uniquely determined. An m-parameter family of potentials exists such that the associated operators have $S(k)$ as their S function and the given quantities $\lambda_n = -\kappa_n^2$ as eigenvalues.

13. OPERATORS WITH M FUNCTIONS DIFFERING BY A RATIONAL FACTOR

The general Gel'fand-Levitan equation was solved in closed form for the case treated in the preceding section. This is not the only situation in which this is possible. It turns out that one may explicitly solve the operator equation for the transformation operator relating two operators L_1 and L_2 whose M functions differ by a rational factor. We shall consider the case where the given operator L_1 with potential $q_1(x)$ has no discrete spectrum, and we shall construct the operator L_2 whose M function is given by

$$M_2(k) = M_1(k) \prod_{l=1}^{N} \frac{k + i\alpha_l}{k + i\beta_l}, \quad \alpha_l > 0, \quad \beta_l > 0. \tag{13.1}$$

The condition $\beta_l > 0$ assures that $M_2(k)$ will be regular in the upper half-plane. The condition $\alpha_l > 0$ does not disturb the generality of the discussion for since

$$\frac{k - i\alpha}{k + i\beta} = \frac{k - i\alpha}{k + i\alpha} \frac{k + i\alpha}{k + i\beta}, \tag{13.2}$$

we may first consider the transformation

$$M(k) = M_1(k)(k - i\alpha)/(k + i\beta), \tag{13.3}$$

and then perform the transformation

$$M_2(k) = M_1(k)(k - i\alpha)/(k + i\alpha), \tag{13.4}$$

as was done in the preceding section.

We shall also assume that the α_l and β_l are all distinct. The equation for the related transformation operator is given by

$$K(x, y) + \Omega(x, y) + \int_0^x K(x, t)\Omega(t, y)\, dt = 0, \qquad y < x, \tag{13.5}$$

$$\Omega(x, y) = \frac{2}{\pi} \int_0^\infty \varphi_1(x, k)[W_2(k) - W_1(k)]\varphi_1(y, k)k^2\, dk$$

$$= \frac{2}{\pi} \int_0^\infty \varphi_1(x, k)W_1(k) \times \left[\prod_{l=1}^{N} \frac{k^2 + \beta_l^2}{k^2 + \alpha_l^2} - 1 \right] \varphi_1(y, k)k^2\, dk. \tag{13.6}$$

If the term in brackets is resolved into partial fractions:

$$\prod_{l=1}^{N} \frac{k^2 + \beta_l^2}{k^2 + \alpha_l^2} - 1 = \sum_{l=1}^{N} \frac{A_l}{k^2 + \alpha_l^2}, \tag{13.7}$$

where

$$A_j = \prod_{l=1}^{N} (\beta_l^2 - \alpha_j^2) \Big/ \prod_{j \neq l}^{N} (\alpha_l^2 - \alpha_j^2), \tag{13.8}$$

then $\Omega(x, y)$ may be expressed in the form

$$\Omega(x, y) = \frac{2}{\pi} \int_0^\infty \varphi_1(x, k) \sum_{l=1}^{N} \frac{A_l}{k^2 + \alpha_l^2} \times W_1(k)\varphi_1(y, k)k^2\, dk = \sum_{l=1}^{N} A_l g_{\alpha_l}(x, y). \tag{13.9}$$

Here, $g_\alpha(x, y)$ is the resolvent kernel of the operator L_1 for $\lambda = -\alpha^2$. In Sec. 2, it was seen that

$$g_\alpha(x, y) = \varphi_1(x, i\alpha)f_1(y, i\alpha)/M_1(i\alpha), \quad x < y, \qquad g_\alpha(x, y) = g_\alpha(y, x), \tag{13.10}$$

is a solution of

$$[-d^2/dx^2 + \alpha^2 + q_1(x)]g_\alpha(x, y) = \delta(x - y). \tag{13.11}$$

Now, any solution of

$$-\psi''(x) - k^2\psi(x) + q_1(x)\psi(x) = 0 \tag{13.12}$$

satisfies

$$(\alpha^2 + k^2) \int_a^b g_\alpha(x, y)\psi(y)\, dy = \psi(x) + [g_\alpha(x, y); \psi(y)]\,|_{y=a}^{y=b}, \tag{13.13}$$

where

$$[\varphi(x); \psi(x)] = \varphi'(x)\psi(x) - \varphi(x)\psi'(x). \tag{13.14}$$

We now seek a solution of (13.5) in the form

$$K(x, y) = \sum_{i=1}^{N} a_i(x)\varphi_i^\beta(y), \tag{13.15}$$

where

$$\varphi_i^\beta(y) = \varphi_1(y, i\beta_i) \qquad (j = 1, \cdots, N). \tag{13.16}$$

The substitution of (13.15) into (13.5) gives

$$\sum_{i=1}^{N} a_i(x)\varphi_i^\beta(y) + \sum_{l=1}^{N} A_l\varphi_l^\alpha(y) \frac{f_l^\alpha(x)}{M_l^\alpha} + \sum_{i=1}^{N} \sum_{l=1}^{N} A_l a_i(x) \int_0^x \varphi_i^\beta(t)g_l^\alpha(t, y)\, dt = 0. \tag{13.17}$$

By (13.13), the last term can be transformed as follows:

$$\sum_{i=1}^{N} \sum_{l=1}^{N} A_l a_i(x) \int_0^x \varphi_i^\beta(t)g_l^\alpha(t, y)\, dt = \sum_{i=1}^{N} \sum_{l=1}^{N} a_i(x) \frac{A_l}{\alpha_l^2 - \beta_i^2} \varphi_i^\beta(y) + \sum_{i=1}^{N} \sum_{l=1}^{N} a_i(x)[g_l^\alpha(x, y); \varphi_i^\beta(x)] \frac{A_l}{\alpha_l^2 - \beta_i^2}. \tag{13.18}$$

The first term in this cancels with the first term in (13.17), and (13.17) may therefore be written as

$$\sum_{l=1}^{N} \frac{A_l \varphi_l^{\alpha}(y)}{M_l^{\alpha}} \left[f_l^{\alpha}(x) + \sum_{i=1}^{N} W_{li}(x) a_i(x) \right] = 0, \quad (13.19)$$

where

$$W_{li}(x) = (\alpha_l^2 - \beta_i^2)^{-1} [f_l^{\alpha}(x); \varphi_i^{\beta}(x)]. \quad (13.20)$$

It is again advantageous to use vector notation. Due to the linear independence of the φ_l^{α}, (13.19) is equivalent to

$$\mathbf{f}(x) + W(x)\mathbf{a}(x) = 0, \quad (13.21)$$

from which it follows that

$$\mathbf{a}(x) = -W^{-1}(x)\mathbf{f}(x) \quad (13.22)$$

and

$$K(x, y) = (\mathbf{a}(x), \boldsymbol{\varphi}(y)) = -(W^{-1}(x)\mathbf{f}(x), \boldsymbol{\varphi}(y)). \quad (13.23)$$

The basic property of the elements of the matrix $W(x)$ is similar to the property (12.10) of the elements of the matrix $V(x)$:

$$dW_{li}(x)/dx = f_l^{\alpha}(x)\varphi_i^{\beta}(x). \quad (13.24)$$

This relation enables one to again obtain elegant expressions for $\Delta q(x)$ and $\varphi_2(x, k)$:

$$\Delta q(x) = -2(d^2/dx^2) \ln ||W(x)||, \quad (13.25)$$

$$\varphi_2(x, k) = \begin{Vmatrix} W(x) & \mathbf{f}(x) \\ \boldsymbol{\beta}(x, k) & \varphi_1(x, k) \end{Vmatrix} \Big/ ||W(x)||, \quad (13.26)$$

where

$$\beta_i(x, k) = \frac{[\varphi_i^{\beta}(x); \varphi_1(x, k)]}{\beta_i^2 + k^2} = \int_0^x \varphi_i^{\beta}(t)\varphi_1(t, k)\, dt. \quad (13.27)$$

The result (13.25) is called Bargmann's formula.

In Sec. 15, it will be shown that $\varphi_2(x, k)$ actually is a solution of (1.1) with the potential $q_2(x) = q_1(x) + \Delta q(x)$. The asymptotic form of $\varphi_2(x, k)$ can be deduced directly from the explicit form of (13.26) just as was done in the preceding section. It is given by

$$\varphi_2(x, k) = (1/(2ik)) \times [M_2(-k)e^{ikx} - M_2(k)e^{-ikx}] + o(1), \quad (13.28)$$

where

$$M_2(k) = M_1(k) \prod_{l=1}^{N} \frac{k + i\alpha_l}{k + i\beta_l}, \quad (13.29)$$

and this proves the correctness of our solution.

The behavior of $\Delta q(x)$ as $x \to 0$ or $x \to \infty$ is easily analyzed. For $x \to 0$, $\Delta q(x)$ decreases exponentially as before, however, $\Delta q(x)$ no longer tends to zero when $x \to 0$. Let us consider one factor for simplicity. From (13.24), we have

$$W(x) = W(0) + \int_0^x f_1(x, i\alpha)\varphi_1(x, i\beta)\, dx. \quad (13.30)$$

But from (13.20), it follows that

$$W(0) = M_1(i\alpha)/(\alpha^2 - \beta^2)$$

and hence

$$W(x) = \frac{M_1(i\alpha)}{\alpha^2 - \beta^2} \left(1 + (\alpha^2 - \beta^2)\frac{x^2}{2}[1 + o(1)]\right), \quad (13.31)$$

$$\Delta q(0) = -2(\alpha^2 - \beta^2). \quad (13.32)$$

The above formulas may be used to determine the potential approximately for a given $S(k)$. Any $S(k)$ may be approximated by a rational function $S_R(k)$. The corresponding approximate function $M_R(k)$ is then given by a product

$$M_R(k) = \prod_{l=1}^{N} \frac{k + i\alpha_l}{k + i\beta_l}. \quad (13.33)$$

The potential constructed from this function can be written in terms of trigonometric functions. Generally speaking, its asymptotic behavior will differ from that of the exact solution. But in some average sense, the behavior of the potential will be described by the approximate solution rather well.

As an example, take the function

$$M(k) = (k + i\alpha)/(k + i\beta). \quad (13.34)$$

The corresponding phase is given by

$$\cot \eta(k) = \frac{\alpha\beta}{\alpha - \beta}\frac{1}{k} + \frac{1}{\alpha - \beta}k, \quad (13.35)$$

and there is no discrete spectrum. For the potential $q(x)$ one obtains

$$q(x) = 2\frac{\beta^2(\beta^2 - \alpha^2)}{(\beta \cosh \beta x + \alpha \sinh \beta x)^2}. \quad (13.36)$$

The expression for $\varphi(x, k)$ is more involved and will not be given.

14. THE CASE $l > 0$

Equation (1.1), heretofore considered, is a particular case of

$$L_v^{(l)} = -y'' + [q(x) + l(l + 1)/x^2]y = s^2 y, \quad (14.1)$$

which results when variables are separated in the three-dimensional Schrödinger equation with a spherically-symmetric potential $q(x)$:

$$-\Delta u + qu = s^2 u. \tag{14.2}$$

In this section, the properties obtained in the preceding sections for the operator L will be extended to the operator $L^{(l)}$. Let

$$\varphi_0^{(l)}(x, s) = (1/s^{l+1}) j_l(sx), \tag{14.3}$$

$$f_0^{(l)}(x, s) = (i)^{l+1} h_l^{(1)}(sx), \tag{14.4}$$

where $j_l(x)$, $h_l^{(1)}(x)$ are spherical Bessel functions. The spherical function corresponding to any cylindrical function is given by

$$z_l(x) = (\tfrac{1}{2}\pi x)^{1/2} Z_{l+1/2}(x) \quad (l = 0, 1, 2, \cdots). \tag{14.5}$$

The above functions behave in the following way:

$$\left.\begin{aligned} \varphi_0^{(l)}(x, s)\,|_{x\to 0} &= \lfloor x^{l+1}/(2l+1)!!][1 + o(1)], \\ \varphi_0^{(l)}(x, s)\,|_{x\to\infty} &= (1/s^{l+1}) \sin(sx - \tfrac{1}{2}l\pi) + o(1), \end{aligned}\right\} \tag{14.6}$$

$$f_0^{(l)}(x, s)\,|_{x\to 0} = [i^l(2l-1)!!/(sx)^l][1 + o(1)],$$

$$f_0^{(l)}(x, s)\,|_{x\to\infty} = e^{isx} + o(1). \tag{14.7}$$

They play roles in the case $l > 0$ analogous to $\sin(sx)/x$ and e^{isx}. The solutions $\varphi^{(l)}(x, s)$ and $f^{(l)}(x, s)$ [the generalizations of $\varphi(x, s)$ and $f(x, s)$], are determined by the conditions

$$\lim_{x\to 0} [(2l+1)!!/x^{l+1}]\varphi^{(l)}(x, s) = 1, \tag{14.8}$$

$$\lim_{x\to\infty} e^{-isx} f^{(l)}(x, s) = 1. \tag{14.9}$$

The integral equations, similar to (1.5) and (1.6) and equivalent to (14.1) with the conditions (14.8) and (14.9), are given by

$$\varphi^{(l)}(x, s) = \varphi_0^{(l)}(x, s) + \int_0^x J^{(l)}(s; x, t) q(t) \varphi^{(l)}(t, s)\, dt, \tag{14.10}$$

$$f^{(l)}(x, s) = f_0^{(l)}(x, s) - \int_x^\infty J^{(l)}(s; x, t) q(t) f^{(l)}(t, s)\, dt. \tag{14.11}$$

Here,

$$J^{(l)}(s; x, t) = (is)^l [\varphi_0^{(l)}(x, s) f_0^{(l)}(t, -s) - \varphi_0^{(l)}(t, s) f_0^{(l)}(x, -s)]. \tag{14.12}$$

By means of these equations, the results of Sec. 1 carry over with respect to the behavior of $\varphi^{(l)}(x, s)$ and $f^{(l)}(x, s)$ in the complex s plane and for large x, etc., under the supposition that the potential $q(x)$ satisfies the condition

$$\int_0^\infty x\, |q(x)|\, dx < \infty. \tag{14.13}$$

Thus, for example, $\varphi^{(l)}(x, s)$ is an entire function of s, $f^{(l)}(x, s)$ is analytic in s in the half-plane $\tau > 0$, and

$$|\varphi^{(l)}(x, s)| \le K\left(\frac{x}{1 + |s|\, x}\right)^{l+1} e^{|\tau| x}, \tag{14.14}$$

$$|f^{(l)}(x, s)| \le K\left(\frac{1 + |s|\, x}{|s|\, x}\right)^{l} e^{-\tau x}, \quad \tau \ge 0, \tag{14.15}$$

For large $|s|$, $f^{(l)}(x, s)$ behaves asymptotically like

$$f^{(l)}(x, s) = e^{isx} + o(1), \qquad \tau \ge 0. \tag{14.16}$$

For real s, $\varphi^{(l)}(x, k)$ can be expressed in terms of $f^{(l)}(x, k)$:

$$\varphi^{(l)}(x, k) = (1/2ik)(1/ik)^l [f^{(l)}(x, k) M^{(l)}(-k) - (-1)^l f^{(l)}(x, -k) M^{(l)}(k)], \tag{14.17}$$

where

$$M^{(l)}(s) = \lim_{x\to 0} \frac{(sx)^l}{i^l(2l-1)!!} f^{(l)}(x, s). \tag{14.18}$$

The function $M^{(l)}(s)$ has the same properties as $M(s)$, enumerated in Lemma 1.6. However, the formula for the normalization constant C_n becomes

$$C_n^{(l)} = \int_0^\infty [\varphi^{(l)}(x, i\kappa_n)]^2\, dx = \frac{\dot{M}(i\kappa_n)}{2i\kappa_n^{l+1}(2l+1)!!} \left[\lim_{x\to 0} \frac{f^{(l)}(x, i\kappa_n)}{x^{l+1}}\right]^{-1}. \tag{14.19}$$

As before, we assume that $M^{(l)}(0) \neq 0$. As earlier, the condition $M^{(l)}(0) = 0$ is not stable, and therefore our restriction is of no consequence. With this assumption, the solution $\varphi^{(l)}(x, 0)$ behaves asymptotically for large x like

$$\varphi^{(l)}(x, 0) = Ax^{l+1}[1 + o(1)]. \tag{14.20}$$

The results concerning the expansion theorem, the existence of transformation operators, and the asymptotic expansion of the solution of the Schrödinger equation for large time all generalize to the present case. Thus, the completeness relation for the eigenfunctions becomes

$$\sum_{n=1}^{m} C_n \varphi_n(x) \varphi_n(y) + \frac{2}{\pi} \int_0^\infty \varphi^{(l)}(x, k) \frac{1}{M^{(l)}(k) M^{(l)}(-k)} \times \varphi^{(l)}(y, k) k^{2(l+1)}\, dk = \delta(x - y). \tag{14.21}$$

Furthermore, the following representations for

$\varphi^{(l)}(x, s)$ and $f^{(l)}(x, s)$ hold:

$$\varphi^{(l)}(x, s) = \varphi_0^{(l)}(x, s) + \int_0^x K^{(l)}(x, t)\varphi_0^{(l)}(t, s)\, dt, \quad (14.22)$$

$$f^{(l)}(x, s) = f_0^{(l)}(x, s) + \int_x^\infty A^{(l)}(x, t)f_0^{(l)}(t, s)\, dt. \quad (14.23)$$

The scattering operator associated with $L^{(l)}$ is determined by the formula

$$S^{(l)}(k) = M^{(l)}(-k)/M^{(l)}(k). \quad (14.24)$$

This same function occurs in the asymptotic representation of the normalized eigenfunction $\psi^{(l)}(x, k) = (ik)^l\varphi^{(l)}(x, k)/M^{(l)}(k)$:

$$\psi^{(l)}(x, k)\,|_{x\to\infty} = \frac{1}{2_i k}\left[S^{(l)}(k)e^{ikx} - (-1)^l e^{-ikx}\right] + o(1). \quad (14.25)$$

As before, these results allow one to solve the inverse problem, i.e., the reconstruction of $L^{(l)}$ from its S function. Thus the kernel $K^{(l)}(x, y)$ satisfies the equation

$$K^{(l)}(x, y) + \Omega^{(l)}(x, y) + \int_0^x K^{(l)}(x, t)\Omega^{(l)}(t, y)\, dt = 0, \quad x > y, \quad (14.26)$$

where

$$\Omega^{(l)}(x, y) = \sum_{n=1}^{m} C_n\varphi_0^{(l)}(x, i\kappa_n)\varphi_0^{(l)}(y, i\kappa_n) + \frac{2}{\pi}\int_0^\infty \varphi_0^{(l)}(x, k)\frac{1}{M^{(l)}(k)M^{(l)}(-k)} \times \varphi_0^{(l)}(y, k)k^{2(l+1)}\, dk. \quad (14.27)$$

By a repetition of our earlier reasoning, this equation can be shown to have a unique solution, and the completeness relation (14.21) can be derived for the functions $\varphi^{(l)}(x, k)$, determined by its solution $K^{(l)}(x, y)$ according to (14.22). Moreover, a differential equation of the form (14.11) can be derived for $\varphi^{(l)}(x, k)$. However, tracing the relationship between $S^{(l)}(k)$ and the potential $q(x)$ by means of Eq. (14.26) or the analog of the Marchenko equation turns out to be difficult. This is due to the fact that the kernel of Eq. (14.26) is expressed in terms of Bessel functions for which there is no simple addition formula such as exists for the trigonometric functions. Of course, conditions such as (6.7) and (6.9) still hold for the S function in the present case. As to the analog of (6.8), it is not clear beforehand that it is convenient to formulate one in terms of the Fourier transform of $S^{(l)}(k)$. One might have thought that the Fourier transform naturally arises in the case $l = 0$ because we are dealing with trigonometric functions. All the more surprising is the fact that the behavior of the S function for $L^{(l)}$ turns out to be no different than that of the S function for $L^{(0)}$. More precisely, we have

Theorem 14.1. *If $S(k)$ is the S function for the operator $L^{(l)}$ associated with the differential equation* (14.1) *with potential $q(x)$, then it is also the S function of an operator $L^{(m)}$ for any $m = 0, 1, 2, \cdots, l + 1, \cdots$, where the corresponding potential $q^{(m)}(x)$ behaves like $q(x)$ as $x \to 0$ and $x \to \infty$.*

The proof of this theorem will be given in the following section. Also, the sense in which the behavior of the potentials $q(x)$ and $q^{(m)}(x)$ is analogous will be made more precise there.

15. TRANSFORMATION OF STURM-LIOUVILLE TYPE EQUATIONS

In the preceding sections, we mentioned repeatedly that a number of statements would be proved in Sec. 15 on the basis of a certain general method. The essence of this method will now be presented from which these statements will then follow.

Let $y_0(x)$ be some particular solution of

$$-y'' + q(x)y = \lambda y \quad (15.1)$$

for $\lambda = \lambda_0$ which does not vanish in the neighborhood of the point $x = a$. Consider the expression

$$y_1(x, \lambda) = [y(x, \lambda); y_0(x)]/[(\lambda - \lambda_0)y_0(x)], \quad (15.2)$$

where $y(x, \lambda)$ is an arbitrary solution of (15.1) and $[\varphi; \psi]$ is the Wronskian of φ and ψ:

$$[\varphi; \psi] = \varphi'(x)\psi(x) - \varphi(x)\psi'(x). \quad (15.3)$$

Lemma 15.1. *The function $y_1(x, \lambda)$ is a solution of* (15.1) *with a potential $q_1(x) = q(x) + \Delta q(x)$, where*

$$\Delta q(x) = -2\frac{d}{dx}\frac{y_0'(x)}{y_0(x)} = -2\frac{d^2}{dx^2}\ln y_0(x). \quad (15.4)$$

To prove this, we note that any two solutions of (15.1) satisfy the equality

$$\frac{d}{dx}\frac{[y(x, \lambda_1); y(x, \lambda_2)]}{\lambda_1 - \lambda_2} = y(x, \lambda_1)y(x, \lambda_2). \quad (15.5)$$

Therefore,

$$y_1'(x, \lambda) = y(x, \lambda) - \frac{[y(x, \lambda); y_0(x)]}{(\lambda - \lambda_0)y_0^2(x)}y_0'(x) = y(x, \lambda) - y_1(x, \lambda)v(x), \quad (15.6)$$

where the function $v(x) = y_0'(x)/y_0(x)$ is a solution of the Riccati equation

$$v'(x) + v^2(x) = q(x) - \lambda_0. \tag{15.7}$$

Differentiating (15.6) once and using (15.2), (15.6), and (15.7), we find that

$$\begin{aligned} y_1''(x, \lambda) &= y'(x, \lambda) - y_1'(x, \lambda)v(x) - y_1(x, \lambda)v'(x) \\ &= y'(x, \lambda) - y(x, \lambda)y_0'(x)/y_0(x) \\ &\quad + y_1(x, \lambda)v^2(x) - y_1(x, \lambda)v'(x) \\ &= -[y(x, \lambda); y_0(x)]/y_0(x) \\ &\quad + y_1(x, \lambda)[v^2(x) + v'(x)] - 2y_1(x, \lambda)v'(x) \\ &= [\lambda_0 - \lambda + v^2(x) + v'(x) - 2v'(x)]y_1(x, \lambda), \end{aligned}$$

i.e.,

$$-y_1''(x, \lambda) + q_1(x)y_1(x, \lambda) = \lambda y_1(x, \lambda). \tag{15.8}$$

This proves the lemma.

Formula (15.2) is meaningful only if $\lambda \neq \lambda_0$. If $\lambda = \lambda_0$, one of the solutions of the transformed equation is

$$z_{10}(x) = 1/y_0(x). \tag{15.9}$$

As a second linearly independent solution, one may take

$$y_{10}(x) = z_{10}(x) \int^x \frac{dt}{z_{10}^2(t)} = \frac{1}{y_0(x)} \int^x y_0^2(t)\, dt. \tag{15.10}$$

Of course, the solutions (15.9) and (15.10) may be deduced from (15.2) by a limiting process. Conversely, the function $y(x, \lambda)$ is expressible in terms of solutions of the transformed equation. For this it suffices to note that (15.9) yields

$$y_0'(x)/y_0(x) = -z_{10}'(x)/z_{10}(x) \tag{15.11}$$

and, therefore, (15.6) can be written in the form

$$\begin{aligned} y(x, \lambda) &= y_1'(x, \lambda) - y_1(x, \lambda)z_{10}'(x)/z_{10}(x) \\ &= [y_1(x, \lambda); z_{10}(x)]/z_{10}(x). \end{aligned} \tag{15.12}$$

This expression defines the transformation inverse to (15.2).

Thus far, we have considered the transformation (15.2) in the neighborhood of $x = a$ where the mapping solution y_0 does not vanish. We now describe the behavior of the solution of the transformed equation when this condition fails to hold. With the application to (1.1) and (14.1) in mind, we shall assume that the singular point occurs at $x = 0$ and that in the neighborhood of $x = 0$, the given potential has the singular behavior

$$q(x) = l(l + 1)/x^2 + O(1/x^{2-\epsilon}), \quad \epsilon > 0. \tag{15.13}$$

This requirement is somewhat stronger than the condition imposed on the potential in Secs. 1 and 14, namely,

$$\int_0^\infty x\, |q(x)|\, dx < \infty, \tag{15.14}$$

but it simplifies considerably all of the calculations. In this case, (15.1) will be said to have an *l singularity* at $x = 0$. Two types of solutions exist in the neighborhood of $x = 0$, one regular:

$$y(x, \lambda) = C(\lambda)x^{l+1}[1 + O(x^\epsilon)], \tag{15.15}$$

and the other irregular:

$$z(x, \lambda) = [D(\lambda)/x^l][1 + O(x^\epsilon)]. \tag{15.16}$$

Evidently, all regular solutions differ only by a factor.

We now perform a transformation using a regular solution $y(x, \lambda_0)$ of (15.1). As a result, to the potential $q(x)$ is added the term

$$\begin{aligned} \Delta q(x) &= -2(d^2/dx^2) \ln x^{l+1}[1 + O(x^\epsilon)] \\ &= 2(l + 1)/x^2 + O\left(\frac{1}{x^{2-\epsilon}}\right) \end{aligned} \tag{15.17}$$

so that the equation has an $(l + 1)$ singularity at $x = 0$. In the derivation of (15.17), the asymptotic representation for $\Delta q(x)$ has been differentiated, but this can be rigorously justified.

Let us observe what happens to a regular and irregular solution under our transformation. By virtue of (15.5) and (15.15)

$$\frac{[y(x, \lambda); y(x, \lambda_0)]}{(\lambda - \lambda_0)} = \int_0^x y(t, \lambda)y(t, \lambda_0)\, dt. \tag{15.18}$$

Therefore,

$$\begin{aligned} y_1(x, \lambda) &= C(\lambda) \int_0^x x^{2(l+1)}[1 + O(x^\epsilon)]\, dx/x^{l+1} \\ &= \frac{C(\lambda)}{2l + 3} x^{l+2}[1 + O(x^\epsilon)]. \end{aligned} \tag{15.19}$$

Furthermore,

$$\begin{aligned} &[z(x, \lambda); y(x, \lambda_0)] \\ &\quad = (2l + 1)\, D(\lambda)C(\lambda_0)[1 + O(x^\epsilon)] \end{aligned} \tag{15.20}$$

so that

$$z_1(x, \lambda) = [(2l + 1)\, D(\lambda)/x^{l+1}][1 + O(x^\epsilon)]. \tag{15.21}$$

In the following, (15.2) will be used to transform a regular solution and (15.12) to transform an irregular one. We have thus shown that under a transformation with a regular solution, the l singularity at the origin is increased by one, and regular and irregular solutions go into regular and irregular

solutions, respectively. It is not difficult to see that transforming with an irregular solution lowers the l singularity of the equation by one but again preserves the nature of the respective solutions.

Thus, to obtain an equation having the same l singularity as the given equation, we must perform two successive transformations, the first using a regular solution of the given equation and the second then using an irregular solution of the transformed equation. It turns out that the transformations constructed in Secs. 12 and 13 by means of the Gel'fand-Levitan equation could be deduced in this way. We illustrate this by transforming two operators whose spectra differ by a single eigenvalue. Consider an equation of type (1.1) with a potential satisfying condition (1.2) and assume that none of the points in the discrete spectrum of the associated operator L lie to the left of $\lambda = -\beta_0^2$. Take some $\beta > \beta_0$. Under our conditions, $\varphi_0(x) = \varphi(x, i\beta)$ vanishes only at $x = 0$. Perform the transformation (15.2) using this solution. Then the transformed equation will have an l singularity at $x = 0$ with $l = 1$. The function

$$\psi_1(x) = \frac{1}{\varphi_0(x)}\left[1 + C\int_0^x \varphi_0^2(t)\,dt\right] \tag{15.22}$$

will be an irregular solution of the transformed equation. Performing a transformation with this solution, we arrive at an equation which has no singularity at $x = 0$. Let us calculate the potential and solution $\varphi_2(x, k)$ associated with this equation. To do this, we must combine the formulas

$$\varphi_1(x, k) = \frac{[\varphi(x, k); \varphi_0(x)]}{(k^2 + \beta^2)\varphi_0(x)} = \frac{1}{\varphi_0(x)}\int_0^x \varphi(t, k)\varphi_0(t)\,dt, \tag{15.23}$$

$$\varphi_2(x, k) = [\varphi_1(x, k); \psi_1(x)]/\psi_1(x), \tag{15.24}$$

$$\Delta q(x) = -2(d^2/dx^2)\ln\varphi_0(x) - 2(d^2/dx^2)\ln\psi_1(x). \tag{15.25}$$

This leads to the following results

$$\varphi_2(x, k) = \varphi(x, k) - \left\{\varphi_0(x)\Big/\left[1 + C\int_0^x \varphi_0^2(t)\,dt\right]\right\} \times \int_0^x \varphi(t, k)\varphi_0(t)\,dt, \tag{15.26}$$

$$\Delta q(x) = -2\frac{d^2}{dx^2}\ln\left[1 + C\int_0^x \varphi_0^2(t)\,dt\right]. \tag{15.27}$$

These formulas correspond exactly to (12.14) and (12.15). Thus by a direct verification, we have shown that the function $\varphi_2(x, k)$ determined by these formulas is a solution of (1.1) with the potential given by (15.25).

To justify the unproved statement of Sec. 13, we now perform the following operations: the transformation of the given equation using the solution $\varphi(x, i\beta)$; the transformation of the resulting equation using the solution $f_1(x, i\alpha)$ obtained from the solution $f(x, i\alpha)$ of the given equation by the first transformation. By combining the formulas

$$\varphi_1(x, k) = \frac{[\varphi(x, k); \varphi(x, i\beta)]}{(k^2 + \beta^2)\varphi(x, i\beta)} = \frac{1}{\varphi(x, i\beta)}\int_0^x \varphi(t, k)\varphi(t, i\beta)\,dt, \tag{15.28}$$

$$f_1(x, i\alpha) = \frac{[f(x, i\alpha); \varphi(x, i\beta)]}{(\beta^2 - \alpha^2)\varphi(x, i\beta)} = \frac{W(x)}{\varphi(x, i\beta)}, \tag{15.29}$$

$$\varphi_2(x, k) = \frac{[\varphi_1(x, k); f_1(x, i\alpha)]}{f_1(x, i\alpha)}, \tag{15.30}$$

$$\Delta q(x) = -2(d^2/dx^2)\ln\varphi(x, i\beta) - 2(d^2/dx^2)\ln f_1(x, i\alpha), \tag{15.31}$$

we find that

$$\varphi_2(x, k) = \varphi(x, k) - \frac{f(x, i\alpha)}{W(x)}\frac{[\varphi(x, k); \varphi(x, i\beta)]}{k^2 + \beta^2} \tag{15.32}$$

is the solution of (1.1) with the potential

$$q_2(x) = q(x) - 2(d^2/dx^2)\ln W(x) = q(x) - 2\frac{d^2}{dx^2}\ln\frac{[f(x, i\alpha); \varphi(x, i\beta)]}{\beta^2 - \alpha^2}. \tag{15.33}$$

This proves the statement of Sec. 13.

The above properties of the transformation will now be used to prove Theorem 14.1. A transformation using any regular solution changes an l singularity only at $x = 0$. The behavior of the potential increment $\Delta q(x)$ as $x \to \infty$ may be different depending on the location of the parameter λ in the complex plane. Thus, in the cases considered till now, the potential increment decreases exponentially as $x \to \infty$. However, there exists solutions which change the singularity of the equation in the same way both for $x \to 0$ and $x \to \infty$. Such a solution is the solution of (15.1) for $\lambda = 0$. If we assume that

$$q(x) = l(l + 1)/x^2 + O\left(\frac{1}{x^{2+\delta}}\right), \quad \delta > 0, \tag{15.34}$$

as $x \to \infty$, then using equations such as (14.10) and (14.11), we can show that the regular solution has the asymptotic representation

$$y(x, 0) = Cx^{l+1}[1 + O(1/x^\delta)]. \tag{15.35}$$

as $x \to \infty$ and among the irregular solutions there exists a $z(x, 0)$ such that

$$z(x, 0) = (D/x^l)[1 + O(1/x^5)] \qquad (15.36)$$

as $x \to \infty$. Under transformations using these solutions,

$$\Delta q(x) = -2(d^2/dx^2) \ln y(x, 0) = 2(l + 1)/x^2 + O(1/x^{2+\delta}), \qquad (15.37)$$

$$\Delta q(x) = -2(d^2/dx^2) \ln z(x, 0) = -2l/x^2 + O(1/x^{2+\delta}). \qquad (15.38)$$

Thus, they have the required property of changing in an identical way the singularity of the equation for $x \to 0$ and $x \to \infty$. Let us see how the S functions change under transformations using these solutions. It is easily verified that the functions

$$f^{(l+1)}(x, k) = -[f^{(l)}(x, k); y(x, 0)]/iky(x, 0), \qquad (15.39)$$

$$f^{(l-1)}(x, k) = -[f^{(l)}(x, k); z(x, 0)]/ikz(x, 0) \qquad (15.40)$$

have the asymptotic behavior

$$f^{(l\pm1)}(x, k) = e^{ikx} + o(1), \qquad (x \to \infty) \qquad (15.41)$$

and are thus solutions of the transformed equations analogous to $f^{(l)}(x, k)$. The function $M(k)$, determining the S function, occurs in the asymptotic formula for the solutions $f^{(l)}(x, k)$ as $x \to 0$:

$$f^{(l)}(x, k)\,|_{x\to0} = [(2l - 1)!!/(kx)^l]i^lM(k)[1 + O(x^\epsilon)]. \qquad (15.42)$$

However, by virtue of (15.20), we find that

$$f^{(l+1)}(x, k)\,|_{x\to0} = [(2l + 1)!!/(kx)^{l+1}]i^{l+1}M(k)[1 + O(x^\epsilon)], \qquad (15.43)$$

$$f^{(l-1)}(x, k)\,|_{x\to0} = [(2l - 3)!!/(kx)^{l-1}]i^{l-1}M(k)[1 + O(x^\epsilon)]. \qquad (15.44)$$

Thus, we have shown that under transformations using the solutions $y(x, 0)$ and $z(x, 0)$, M and, hence, the S function remain unchanged. This result together with formulas (15.17), (15.37), and (15.38) for the asymptotic behavior of the potential as $x \to 0$ and $x \to \infty$, proves Theorem 14.1.

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APPENDIX (COMMENTS AND NOTES ON THE LITERATURE)

1. The proofs of Lemmas 1.1–1.3 and 1.5 are found in Levinson's paper.[7] Certain of the statements are proved by Jost[33] and by Bargmann.[34] The case $M(0) = 0$ is treated in detail by Marchenko and Agranovich.[35,36]

2. The completeness theorem for the eigenfunctions of the operator L in the form (2.6) is proved by Levinson[7] for the case of no discrete spectrum. The general case is considered by Jost and Kohn.[12]

3. Many papers have been devoted by both physicists and mathematicians to the question of how the solution of the time dependent Schrödinger equation behaves for large $|t|$. A nonrigorous proof of the existence of the limits of the operator $U(0, t) = e^{iLt}e^{-iL_0t}$ as $t \to \pm\infty$, typical of physics papers, is given for example, in the survey of Gellmann and Goldberger.[37] From mathematical work, it is necessary to mention first of all the articles of Friedrichs,[26] who proved the existence of $\lim_{|t|\to\infty} U(0, t)$. He also showed that the limiting operators are unitary for a wide class of unperturbed operators L_0 on the assumption that the perturbation operator V is small. A formal presentation of his method appears in the paper of Moses.[38] Cook[39] proved the existence of $\lim_{|t|\to\infty} U(0, t)$ for the three-dimensional operator $-\Delta u + q(x)u$ assuming only that $q(x)$ is square integrable over all of space. However, he did not study the question of whether the operator $S = U(0, \infty)^*U(0, -\infty)$ is unitary. The restriction that the perturbation operator V be small is removed in the paper of Ladizhenskaya and Faddeyev[40] using the formalism of Friedrichs.

Theorem 3.1 does not follow from the results of these papers under the conditions we have imposed on the potential $q(x)$. The elementary proof cited makes use of the concrete properties of the example under consideration and does not carry over to other problems.

4. Povzner[41] and Levitan[42] first obtained and used the representation (4.3) for $\varphi(x, k)$. Formula (4.2)

[33] R. Jost, Helv. Phys. Acta **20**, 256 (1947).
[34] V. Bargmann, Revs. Modern Phys. **21**, 488 (1949).
[35] Z. S. Agranovich and V. A. Marchenko, Doklady Akad. Nauk S. S. S. R. **113**, 951 (1957).
[36] Z. S. Agranovish and V. A. Marchenko, *The Inverse Problem in the Quantum Theory of Scattering*, Izd. Kharkov Univ., 1960. (An English translation in preparation).
[37] M. Gellman and M. Goldberger, Phys. Rev. **91**, 398 (1953).
[38] H. E. Moses, Nuovo cimento **1**, 103 (1955).
[39] J. M. Cook, J. Math. and Phys. **36**, 83 (1957).
[40] O. A. Ladizhenskaya and L. D. Faddeyev, Doklady Akad. Nauk S.S. S. R. **120**, 1187 (1958).
[41] A. Ya. Povzner, Matem. Sbornik. **23**, 3 (1948).
[42] B. M. Levitan, Uspekhi Math. Nauk **4**, 3–112 (1949).

for $f(x, k)$ was deduced by Levin[43] and our first derivation repeats his argument. The method of deriving the integral equations (4.4) and (4.5) and the inequalities (4.7) and (4.8) is due to Agranovich and Marchenko.[35,36]

The theorem of Titchmarsh mentioned can be formulated in the following way: A necessary and sufficient condition for $\Phi(x)$ to be the limit of some function $\Phi(z) = \Phi(x + iy)$, which is analytic in the upper half-plane and such that

$$\int_{-\infty}^{\infty} |\Phi(x + iy)|^2 \, dx = O(e^{-2ky}),$$

is that

$$\varphi(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Phi(x) e^{-ixt} \, dx = 0, \qquad t < k.$$

5. The general concept of transformation operator, as already noted, was developed by Friedrichs.[25,26] Some of the notation and the proof of Theorem 5.2 were taken from the articles of Kay and Moses[21,23] who applied Friedrichs' method in solving inverse problems.

From the formula (5.15) for the S function, it follows that $S(k)$ cannot, in general, be continued into the complex k plane. Thus, Heisenberg's supposition that the discrete energy levels for the example in question might be determined by the analytic continuation of the S matrix is not justified. This fact was noted by Jost.[33]

The differential equation (5.25) with the condition (5.24) is the starting point for the proof of the existence of the kernel $K(x, y)$ in the paper of Gel'fand and Levitan.[15] One easily obtains the integral equation (4.4) from this equation. Chudov[44] proposed using the nonlinear equation, obtained from (5.25) by replacing $q(x)$ by $2\, dK(x, x)/dx$, to solve the inverse problem. Giving the S function for large x provides Cauchy data for this equation.

6. The method of relating $W(k)$ and $S(k)$ on the basis of the Wiener-Levi theorem is due to Krein.[19,45] The Wiener-Levi theorem can be stated in the following way. Let the function $\Phi(z)$ be analytic in a region D and then let $F(\lambda)$ be so chosen that the curve $z = F(\lambda)$ $(-\infty \leq \lambda \leq \infty)$ lies inside D. If $F(\lambda)$ is representable in the form

$$F(\lambda) = C + \int_{-\infty}^{\infty} f(t) e^{i\lambda t} \, dt,$$

where $f(t)$ is absolutely integrable, then $\Phi(F(\lambda))$ also possesses this property.

Formula (6.9) was deduced by Levinson[7] and bears his name.

7. The relationship between the kernels $K(x, y)$ and $A(x, y)$ does not appear in the literature.

8. The first derivation of (8.5) is taken from the paper of Kay and Moses.[21] The derivation of the general equation (8.14) follows the reasoning of Gel'fand and Levitan.[15]

9. The existence proof for (8.14) is taken from the paper of Jost and Kohn[16] and to a great extent follows the reasoning of Gel'fand and Levitan. The subsequent presentation with certain modifications reproduces the arguments of Kay and Moses.[21]

10. The analysis of the properties of the potential $q(x)$ is taken from the monograph of Agranovich and Marchenko.[36] The various relationships between $q(x)$ and $W(k)$ or $S(k)$ were obtained by Neuhaus,[46] Friedman, [47] Jost,[48] and Newton.[49] However the more general results follow from (10.11) and (10.24).

11. Krein's methods are given in a series of articles[50,51,19,and52] (see also his lectures presented at MGU in 1956–1957). Only certain of his results are mentioned in the survey. The system of differential equations (11.19) is the starting point of Krein's methods.

12. Formula (12.14) for the increment in the potential was obtained by Jost and Kohn.[16] The simplest formula for the solution $\varphi(x, k)$, such as (12.15), is due to Krein[19] (for the case $m = 1$).

The portion of Theorem 12.1 concerning necessary and sufficient conditions is due to Marchenko and Agranovich.[35,36]

13. In solving (13.5), we have followed the paper of Fulton and Newton[53] who refer to the work of Bargmann as the source of the method used. Expression (13.25) is called Bargmann's formula. Formulas for $\varphi(x, k)$ such as (13.26) are cited by Theiss.[54]

Another approach to the problem was developed

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[43] B. Ya. Levin, Doklady Akad. Nauk S. S. S. R. **106**, 187 (1956).
[44] L. A. Chudov, Izd. OIYaI, (1958).
[45] M. G. Krein, Integral equations on a half-line with difference type kernels, Uspekhi Math. Nauk. **13**, 3 (1958).
[46] M. G. Neuhaus, Doklady Akad. Nauk S.S.S.R. **102**, 25 (1955).
[47] B. Friedman, Michigan Math. J. **4**, 137 (1957).
[48] R. Jost, Helv. Phys. Acta **29**, 410 (1956).
[49] R. G. Newton, Phys. Rev. **101**, 1588 (1956).
[50] M. G. Krein, Doklady Akad. Nauk S.S.S.R. **94**, 987 (1953).
[51] M. G. Krein, Doklady Akad. Nauk S.S.S. R. **97**, 21 (1954).
[52] M. G. Krein, Doklady Akad. Nauk S.S.S.R. **111**, 1167 (1956).
[53] T. Fulton and R. G. Newton, Nuovo cimento **3**, 677 (1956).
[54] W. R. Theis, Z. Naturforsch. **11a**, 889 (1956).

by Krein if $M_1(k) = 1$. His results are formulated in a definitive way in reference 55, the formulas there being simpler than (13.25) and (13.26). However, these formulas are not generalized to the case $M_1(k) \neq 1$.

14. The basic properties of solutions of (14.1) for $l > 0$ are obtained by Levinson,[7] by Jost and Kohn,[16] and by Newton.[56] The papers of Stashevskaya[57] and Volk[58] are devoted to carrying over the results of Gel'fand and Levitan to equations with a singularity at $x = 0$. Theorem 14.1 is due to Marchenko (it was presented at the April, 1956 meeting of the Kharkov Mathematical Society).

15. A transformation such as (15.2) was first applied by Crum,[59] who used it to change a differential operator defined over a finite interval into an operator having one less eigenvalue than the original operator. Krein extended Crum's method and applied the results to get a complete characterization of the spectral function of an equation with the singularity $l(l+1)/x^2$ in the potential at $x = 0$. Marchenko made use of an analogous transformation to analyze the relationship between the S function and a potential given by

$$q(x) = q_1(k) + \frac{l(l+1)}{x^2}, \quad \int_0^\infty x^{1+\varepsilon} |q_1(x)|\, dx < \infty.$$

The presentation in the survey differs somewhat from the methods of the above-mentioned authors.

It is interesting to note that since the formulas (12.14), (12.15) and (13.25), (13.26) are verified by algebraical means without recourse to the properties of the general Gel'fand-Levitan equation, they still hold for complex values of the parameters κ_n, C_n, α_l, and β_l. The associated potential is, generally speaking, a complex function with a singularity of the form $m(m+1)/(x-x_0)^2$ at any point where $\|V(x)\| = 0$ or $\|W(x)\| = 0$, in which m is the multiplicity of any such existing zero. This fact was noted by Krein[19] and by Theiss.[54]

We now briefly consider some of the generalizations of the problem investigated in our survey. By analyzing many of the formulas in the text, one sees that they remain valid with appropriate changes for systems of equations, i.e., for the matrix generalization of (1.1):

$$-Y'' + Q(x)Y = k^2 Y.$$

Here, $Q(x)$ is a real symmetric matrix. The solutions $\varphi(x, k)$, $f(x, k)$ and the functions $W(k)$, $M(k)$, and $S(k)$ now become matrices. Therefore it is necessary to pay attention to the order of factors in generalizing formulas to the matrix case. The matrix $M(s)$ is analytic in the upper half-plane $\tau > 0$ and singular at those points corresponding to the discrete spectrum. The matrices $W(k)$ and $S(k)$ are related to it by the formulas

$$W(k) = M(k)^{-1}M^T(-k)^{-1}, \quad S(k) = M(-k)M^T(k)^{-1},$$

$M^T(k)$ being the transposed of $M(k)$. Similar systems were studied by Jost and Newton,[60] by Krein,[52] and by Agranovich and Marchenko.[35,36] A fundamental difficulty arises in carrying over the discussion of Sec. 6 to the matrix case. In consequence of the noncommutativity of the matrices, the formulas cited there no longer hold. To find how $W(k)$ and $S(k)$ are related, one has to go back and consider integral equations of the form

$$K(t) = F(t) + \int_0^\infty F(t+s)K(s)\, ds.$$

Marchenko and Agranovich derived necessary and sufficient conditions on the S matrix so that it corresponds to a matrix potential $Q(x)$ from a given class making use of analogous integral equations. The formulation of conditions directly in terms of the S matrix still remains an unsolved problem.

Newton[56] and Agranovich and Marchenko[36,61] considered a system in which the potential has the singularity $l_\alpha(l_\alpha+1)\delta_{\alpha\beta}/x^2$; Agranovich and Marchenko reduced such a system to a regular one by transformations generalizing those introduced in Sec. 15.

The inverse problem for a system has mainly been treated for the purpose of seeing what means are needed to solve the inverse problem for the Schrödinger equation

$$-\Delta u + q(x)u = k^2 u$$

in all of space when the potential decreases in all directions. However, this problem essentially differs from those treated till now. In fact, the S matrix in this case is determined by the so-called scattering amplitude $f(k; \alpha, \beta)$ depending on the wave number $k (0 \leq k < \infty)$ and two unit vectors α and β. Thus, the S matrix depends on a larger number of parameters than the potential $q(x)$ which may be regarded

[55] M. G. Krein, Doklady Akad. Nauk S.S.S.R. **113**, 970 (1957).
[56] R. G. Newton, Phys. Rev. **100**, 412 (1955).
[57] V. V. Stashevskaya, Doklady Akad. Nauk S.S.S.R. **93**, 409 (1953).
[58] V. Ya. Volk, UMN VIII, 141 (1953).
[59] M. M. Crum, Quart. J. Math. **6**, 121 (1955).
[60] R. G. Newton and R. Jost, Nuovo cimento **1**, 590 (1955).
[61] Z. S. Agranovich and V. A. Marchenko, Doklady Akad. Nauk S. S. S. R. **118**, 1055 (1958).

as a function of the distance $r(0 \leq r < \infty)$ and one unit vector. In this sense, the problem is over determined and it is necessary to look for non-trivial properties of the S matrix which would decrease the number of parameters on which it depends.

The simplest analogous problem arises in the reconstruction of a decreasing potential from the S matrix for the one-dimensional Schrödinger equation

$$-y'' + q(x)y = k^2 y \qquad (-\infty < x < \infty).$$

In this case, the S matrix is a 2×2 matrix:

$$S(k) = \begin{bmatrix} s_{11}(k) & s_{12}(k) \\ s_{21}(k) & s_{22}(k) \end{bmatrix} = \begin{bmatrix} a(k) & b(k) \\ b(k) & c(k) \end{bmatrix},$$

and due to its unitariness, is determined by giving three real functions of $k(0 \leq k < \infty)$. The potential may be regarded as being given by two real functions of $x(0 \leq x < \infty)$.

The inverse problem for this case was considered by Kay and Moses[23,24] (as an example illustrating their general approach to the inverse problem) and by the author.[62] In reference 62 it is shown that an additional condition on the S matrix follows from the analyticity of the coefficient $b(k)$ in the upper half-plane $\tau > 0$. This condition implies that the whole S matrix (and potential) is determined by one of the coefficients $a(k)$ or $c(k)$ which may be chosen as an arbitrary function. The reconstruction of the equation with an arbitrary potential from its spectral matrix function was treated by Bloch.[63]

A number of the elements of the S matrix are also analytic in the three-dimensional case. The proof of this fact is given in the papers of Khuri[64] and of the author[65] in connection with the so-called dispersion relations. However, these relations do not sufficiently reduce the number of parameters on which the S matrix depends.

It is interesting to note, in this connection, the statement of the three-dimensional inverse problem as proposed by Moses[66]: Determine the potential $q(x)$ from the back scattering amplitude $g(k, \alpha) = f(k; \alpha, -\alpha)$ where α is a vector running over a hemisphere. This data, namely two real functions of $k(0 \leq k < \infty)$ and α, involve as many parameters as does the potential. It is very plausible that the process of Moses converges for sufficiently small $g(k, \alpha)$ which in other respects may be a quite arbitrary function.

A number of papers exist in which the inverse problem has been solved for the relativistic equations when the latter reduce to ordinary differential equations. The equation obtained by separating variables in the Klein-Gordon equation was studied by Corinaldesi.[67] The one-dimensional Dirac equation was considered by Kay and Moses,[68] Toll and Prats,[69] and Verdi.[70] In all of these papers, a relationship is established between the asymptotic phase and the potential both for positive and negative energies. The data, just as in the problems described above, depends on a larger number of parameters than does the potential. A correct formulation of the problem for the radial relativistic equation has still to be given.

[62] L. D. Faddeyev, Doklady Akad. Nauk S.S.S.R. **121**, 63 (1958).
[63] A. Sh. Bloch, Doklady Akad. Nauk S.S.S.R. **92**, 209 (1953).
[64] N. N. Khuri, Phys. Rev. **107**, 1148 (1957).
[65] L. D. Faddeyev, Zhur. Eksptl 'i Teort Fiz **35**, 433 (1958).
[66] H. E. Moses, Phys. Rev. **102**, 559 (1956).
[67] E. Corinaldesi, Nuovo cimento **11**, 468 (1954).
[68] H. E. Moses, Bull. Am. Phys. Soc. **4**, 240 (1957).
[69] J. S. Toll and F. Prats, Phys. Rev. **113**, (1959).
[70] M. Verdi, Nuclear Phys. **9**, 255 (1958/59).

The Line Shape in a Harmonic Lattice

ROBERT ENGLMAN
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts
AND
PERETZ LEVI*
Department of Physics, Technion–Israel Institute of Technology, Haifa, Israel
(Received 18 May 1962)

A general formalism is developed for the treatment of lattice vibrations. The problem is reduced to the mathematics of noncommuting operators. Hausdorff's equation is then solved for a lattice interacting with linear forces. The cases treated in detail are the line shapes of a radiating atom as affected by the displacement (Franck-Condon effect) and by the nuclear recoil (Mössbauer effect). Only formal results are obtained, which are more difficult to compute than those of the method of normal modes. However, they are more general and do not require the data of vibrational frequencies.

1. INTRODUCTION

THIS paper contains a mathematical description of two distinct aspects of the interaction of the lattice with one of its constituent atoms or ions that is emitting or absorbing radiation. The two aspects are those which originate from the instantaneous recoil of the radiating atom or, alternatively, from the instantaneous rearrangement of the neighboring atoms generally due to the changed electronic state of the radiating atom. These two phenomena have come to be known as the nuclear-recoil or Mössbauer effect[1] and the Franck-Condon effect,[2,3] respectively. Though they require the same mathematical formalism for solution, they dominate entirely different physical situations: the first in gamma-ray emission, the second in electronic transitions, as examples. The spirit of this work therefore requires omission of references to the background or to the significance of these effects and also requires that the underlying physical assumptions be dealt with but briefly.

The quantity which will be calculated is the Fourier transform of the spectral line for an ionic crystal held together by harmonic forces of quite general variety. The classic treatment of this problem goes back to 1939.[4] This was more recently applied to the Mössbauer effect by Visscher[5] and, in a modified form, by Lipkin[6] and to the Franck-Condon situation by Pryce[7] and Koide.[8] By all but the last investigator, considerable attention was paid to the "precursor," the sharp line corresponding to no-phonon excitation, which precedes the broad absorption line. A comparison of the present approach with Lamb's method[4] will be made after the derivation of the results. Now it should merely be said that ours is effectively a time-dependent approach, in that we consider the spread of the disturbance around the radiating ion onto farther regions of the crystal. We do not make the transformation to normal coordinates but stay consistently within the mathematical framework of the harmonic Hamiltonian, not resorting to (nor utilizing), as one does in the method of normal modes, some empirical rule about the distribution of frequencies in a solid. In some sense, the present treatment is also more general.

The final result of this work is given in Sec. 9 [Eq. (29)]. The mathematics, which is used on the way, contains some standard techniques in new apparel, such as the finding of the generating function for a random walk with complex probabilities and the folding of Fourier series and asymptotics. On the other hand, the section introducing the Hausdorff formulas for noncommuting operators may be new to the reader, and so will be the method of derivation of the fundamental differential equations in Sec. 5 (these are really difference equations in disguise). It may be said that these equations constitute the crucial stage in the formulation, since they enable us to replace (for our special cases) the hopelessly complicated formula (4) by the closed expressions (9), (10), and (11).

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[1] R. L. Mössbauer, Z. Physik **151**, 124, (1958); Naturwissenschaften **45**, 538, (1958); Z. Naturforsch. **14a**, 211 (1959).
[2] K. Huang and A. Rhys, Proc. Roy. Soc. (London) **A204**, 413 (1951).
[3] M. Lax, J. Chem. Phys. **20**, 1752 (1952).
[4] W. E. Lamb, Jr., Phys. Rev. **55**, 190 (1939).
[5] W. M. Visscher, Ann. Phys. (N. Y.) **9**, 194 (1960).
[6] H. J. Lipkin, Ann. Phys. (N. Y.) **9**, 332 (1960).
[7] M. H. L. Pryce (private communication 1957).
[8] S. Koide, Z. Naturforsch. **15a**, 123 (1960).

The major portion of the argument is carried through for a chain, a one-dimensional lattice. This is extended to a monatomic lattice in Sec. 9; the last stage of generalization, the general harmonic crystal, is treated in Sec. 10.

2. SPECTRAL INTENSITY

Our point of departure is the Fourier transform (variable t), taken with respect to the energy, of the spectral intensity. (We use units in which $\hbar = 1$.) The energy considered is that due to the lattice motion alone. This can be defined precisely only if one assumes the separability of the transition matrix into factors involving the internal (electronic or nuclear) and external coordinates (e.g., the momenta and positions of the nuclei of the lattice). This assumption is commonly made in the literature of the problem and is beyond doubt for nondegenerate internal states. (For degenerate states the Jahn-Teller effect will operate[9] with varying and hitherto unknown effect.) Within the context of this assumption, we say that we take the zero of the spectrum to be the difference between the lowest energies belonging to the two internal states, minus the zero point motion of the lattice. In the configuration diagram, the origin is the vertical distance between the tips of the hyperparaboloids.

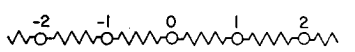
When the intensity is normalized to unity, its Fourier transform may be written as

$$g(t) = \mathrm{Tr}\, e^{itH_f} e^{-(it+\beta)H_i} / \mathrm{Tr}\, e^{-\beta H_i}, \quad (\beta = 1/kT). \quad (1)$$

The Hamiltonian operators H_i and H_f corresponding to the state of the lattice before and after radiation will be given in detail presently. This form, or its equivalent, has been given by Lax[3] and by Koide[8] for the Franck-Condon effect. Investigators of the Mössbauer effect (they are listed at the beginning of the paper) have also worked with equivalent formulas or, as Lamb,[4] with formulas that can be reduced to such after Fourier transformation and standard manipulations.

In Sec. 9 we write down the Hamiltonians for a simple-cubic lattice held together by harmonic forces between nearest, first, and second next neighbors. These are necessarily rather lengthy, but possess no difficulties in principle that are not already exhibited by a linear chain. This is the model we consider now.

3. THE LINEAR CHAIN



$$H_i = \cdots - \frac{1}{2m}\frac{\partial^2}{\partial x_{-1}^2} - \frac{1}{2m}\frac{\partial^2}{\partial x_0^2} - \frac{1}{2m}\frac{\partial^2}{\partial x_1^2} - \cdots + \tfrac{1}{2}m\omega^2(x_{-1} - x_0)^2 + \tfrac{1}{2}m\omega^2(x_0 - x_1)^2 + \cdots .$$

The H_f's are defined as the transforms of H_i, i.e., SH_iS^{-1}, where S is the transformation matrix of the configurational wavefunctions. The H_f's depend on the internal states parametrically. It is much easier, however, to write down H_f simply intuitively, by considering the Hamiltonian which obtains for the lattice with the final internal states.

Three cases apply:

$$\text{(I)} \quad H_f = \cdots - \frac{1}{2m}\frac{\partial^2}{\partial x_{-1}^2} + \frac{1}{2m}\left(-i\frac{\partial}{\partial x_0} + k\right)^2 - \frac{1}{2m}\frac{\partial^2}{\partial x_1^2} \cdots + \tfrac{1}{2}m\omega^2(x_{-1} - x_0)^2 + \tfrac{1}{2}m\omega^2(x_0 - x_1)^2 + \cdots .$$

Because of the momentum balance between the radiation and the radiative ion (labeled by 0) the latter has a recoil momentum $-k$. There is a definite (quantum mechanical) probability[10] that owing to the coupling with the infinite chain, this instantaneous momentum change will be a virtual one; that is, it will not be associated with a change in energy of the ion.

$$\text{(II)} \quad H_f = \cdots - \frac{1}{2m}\frac{\partial^2}{\partial x_{-1}^2} - \frac{1}{2m}\frac{\partial^2}{\partial x_0^2} - \frac{1}{2m}\frac{\partial^2}{\partial x_1^2} - \cdots + \tfrac{1}{2}m\omega^2(x_{-1} - x_0 + a)^2 + \tfrac{1}{2}m\omega^2(x_0 - x_1 + a)^2 + \cdots .$$

The equilibrium distance between the radiating ion and its immediate neighbors is displaced by an amount a. This change is symmetric about the ion, provided the electronic states in the transition will possess definite parities. This is generally so to a good approximation.

Here again, there exists a definite probability that the coupling with the lattice will preclude any real change in the lattice potential energy.

$$\text{(III)} \quad H_f = \cdots - \frac{1}{2m}\frac{\partial^2}{\partial x_{-1}^2} - \frac{1}{2m}\frac{\partial^2}{\partial x_0^2} - \frac{1}{2m}\frac{\partial^2}{\partial x_1^2} - \cdots + \tfrac{1}{2}m\omega'^2(x_{-1} - x_0)^2 + \tfrac{1}{2}m\omega'^2(x_0 - x_1)^2 + \cdots .$$

[9] J. H. Griffiths, *The Theory of Transition-Metal Ions* (Cambridge University Press, New York, 1961).

[10] For an infinite *linear chain* this probability is infinitesimal, while for a crystal it is finite. This is shown later.

A change in the electronic state will in general also change the coupling constants ω of the radiating ion. Changes which may possibly occur farther away (in case II as well) can reasonably be disregarded at this stage.

We do not consider effect III in this work, for the simple reason that it is not amenable to the mathematical treatment which we apply to I and II. It has been considered by Koide[8] and by Englman,[11] by the latter from the point of view that the changed coupling constants introduce localized vibrational modes with frequencies just outside the continua. Its neglect here derives from the hope that the effects of II and III, which *could* occur together, are on the spectral line, qualitatively speaking, independent and additive.

The nuclear recoil and the displacement effects are mathematically characterized by the fact that H_f differs from H_i by a term linear in the dynamical variables and a constant term. For future reference we write this as

$$itH_f = itH_i + \frac{t}{m} k \frac{\partial}{\partial x_0} + it\frac{k^2}{2m} \tag{2.I}$$

$$itH_f = itH_i + itm\omega^2 a(x_{-1} - x_1) + itm\omega^2 a^2. \tag{2.II}$$

4. THE HAUSDORFF FUNCTION

We shall now examine the function $C = C(A, B)$ in the equation $e^A e^B = e^C$, where A and B are noncommuting operators. We first consider the general case, following Hausdorff's paper[12] with some change of notation. The same problem was considered, less completely, by Baker[13] and Campbell.[14] After the general treatment we proceed to calculate C for the special case contained in the above two equations and Eq. (1).

Hausdorff proved the remarkable property of C (in the general case), that it can be written down as a series in the successive order commutators of A and B. In fact, up to the fourth-order commutator

$$\begin{aligned} C = {} & A + B + \tfrac{1}{2}A\cdot B + \tfrac{1}{12}A\cdot B^2 \\ & + \tfrac{1}{12}B\cdot A^2 + \tfrac{1}{24}B\cdot A^2B - \tfrac{1}{720}A\cdot B^4 \\ & - \tfrac{1}{720}B\cdot A^4 + \tfrac{1}{360}A\cdot B^3A + \tfrac{1}{360}B\cdot A^3B \\ & - \tfrac{1}{120}A\cdot B^2AB - \tfrac{1}{120}B\cdot A^2BA + \cdots \end{aligned} \tag{3}$$

where

$$A\cdot B = [A, B],$$

$$A\cdot B^2 = [[A, B], B]$$

$$B\cdot A^2B = [[[B, A], A], B], \text{ etc.}$$

(The dot notation $A\cdot B^n$ is preferred to the notation $\{A, B^n\}$, which is sometimes also used, for typographical reasons and because the curly brackets often mean anticommutation in quantum mechanics.) Note that (this is Hausdorff's point!) C does not contain products of commutators (e.g., $[A, B][A, B]$) but only commutators.

An expression for C as a power series in A may be generated from the relation

$$A\,\mathfrak{D}_A C = \{A\cdot[B(1 - e^{-B})^{-1} - 1] + A\}\,\mathfrak{D}_B C, \tag{4}$$

where $X\mathfrak{D}_A C$ means: Put X successively for each A as this occurs in C.

Examples:

$$X\,\mathfrak{D}_A A^2 = XA + AX,$$

$$A\,\mathfrak{D}_A B\cdot A^3 = 3B\cdot A^3,$$

$$B\,\mathfrak{D}_A A\cdot BA = B\cdot BA + A\cdot BB = A\cdot B^2$$

since $B\cdot B\cdots$ is zero.

On the right-hand side of (4) the content of the square brackets is understood to be the expansion in a power series of B. Note also that $A \neq A\cdot 1 = 0$.

It can be verified with some labor that up to fourth order, the solution (3) is gotten by iterating Eq. (4) and manipulating the result to bring it to the form of commutators. In principle, this procedure can be continued to any desired order, but the labor becomes rapidly excessive. No closed expression or general formula for the coefficients of the commutators is known to exist for general A and B.

The operators A and B with which we are concerned in (1) and (2) are characterized by

$$A = \rho B + (tk/m)(\partial/\partial x_0) + itk^2/2m, \tag{5.I}$$

$$A = \rho B + itm\omega^2 a(x_{-1} - x_1) + itm\omega^2 a^2, \qquad \rho = -(1 - i\beta/t)^{-1}. \tag{5.II}$$

We shall now postulate a type of solution for C in closed form, convert the operational equation (4) into two differential equations and solve these exactly. Put

$$C' = A + B + \tfrac{1}{2}A\cdot B + A\cdot BF(B, \rho)B + A\cdot BG(B, \rho)A, \tag{6}$$

[11] R. Englman, Phil. Mag. **5**, 691 (1960).
[12] F. Hausdorff, Ber. Verhandl. sächs. Akad. Wiss. Leipzig, Naturw. Math-Kl. **58**, 19 (1905).
[13] H. F. Baker, Proc. London Math. Soc. **34**, 91 (1902).
[14] J. E. Campbell, Proc. London Math. Soc. **28**, 381 (1897); **29**, 14 (1898).

where the functions F and G (to be found) are purported to be power series in the operator B and the number ρ.

Why is a closed solution for C' possible? The answer lies in H_i being a quadratic form of the variables and H_f differing from H_i only by a term linear in the variables and a constant term. It follows that the commutators of any degree containing H_f and H_i in any permutation whatever will consist of terms linear of the variables (positions or momenta) and of constant terms. There is now one simple but crucial fact to be taken into account. It is that the replacement of H_f by H_i in a commutator such as

$$H_f \cdot H_i H_i \cdots H_f H_i \cdots H_f$$

is of consequence only in the first place (i.e., before the "dot") or in the last place. If we make a replacement of the first H_f by H_i, we get, of course, zero. If we replace the H_f in the last position, it is the constant term, if there is one, which is removed; everything else is unaffected. This is seen at once if we consider that at the penultimate stage of working, there are linear terms and a constant. This last gives no contribution at the next stage, the former gives rise to linear terms and a constant term when forming the commutator with quadratic and linear terms, respectively. Thus we see that substituting H_i for H_f in the last position results in the deletion of the constant term. This argument also proves that the intermediate H_f may be replaced by H_i. As regards the operators A, B, from (5) we see that in the intermediate positions A may be replaced by ρB (ρ a c-number). Thus the form (6) postulated for C is regarded as established.

5. THE DIFFERENTIAL EQUATION

To find a differential equation for the functions F and G we concentrate on a representative term $A \cdot B\ (\rho^n B^m)B$ in the expression for C. Clearly, before the replacement $A \to \rho B$, this term was one of those terms in C which contained in the intermediate positions nA's and $(m - n)B$'s in some order. Therefore,

$$A\mathfrak{D}_A \text{ (one such term)} = (n + 1) \text{ (this term)}$$
$$\to (n + 1)A \cdot B(P^n B^m)B = (\partial/\partial\rho)\rho[A \cdot B(\rho^n B^m)B].$$

In this manner we find that

$$A\ \mathfrak{D}_A C \to A + \tfrac{1}{2}A \cdot B + (\partial/\partial\rho)A \cdot BF(B, \rho)B + (1/\rho)(\partial/\partial\rho)\rho^2 A \cdot BG(B, \rho)A.$$

This constitutes the replacement of the substitutional operator by a differential one. For the conversion of the right-hand side of (4) we again examine in C a term which becomes $A \cdot B(\rho^n B^m)B$ on the substitution $A \to \rho B$ at intermediate places. Consider first $A\mathfrak{D}_B C$. When the operator $A\mathfrak{D}_B$ is applied to the B's in intermediate positions, the result after the replacement $A \to \rho B$ is clearly $(m - n)A \cdot B(\rho^{n+1} B^m)B$, since there were $(m - n)B$'s originally present in intermediate positions in C and an extra ρ is got as an additional A is introduced. Also

$$(m - n)A \cdot B(P^{n+1} B^m)B = \rho A \cdot B^2[(\partial/\partial B)(\rho^n B^m)]B - \rho^2 A \cdot B(\partial/\partial\rho)(\rho^n B^m)B$$

is another differential expression. The operator $A\mathfrak{D}_B$ acting on the last B yields $A \cdot B(\rho^n B^m)A$, whereas acting on the B immediately after the dot gives zero. We thus obtain

$$A\ \mathfrak{D}_B C \to A + \rho A \cdot B^2[(\partial/\partial B)F(B, \rho)]B + A \cdot BF(B, \rho)A - A \cdot B\rho^2 \frac{\partial}{\partial\rho} F(B, \rho)B + \rho A \cdot B^2\left[\frac{\partial}{\partial B} G(B, \rho)\right]A - A \cdot B\rho^2(\partial/\partial\rho)G(B, \rho)A.$$

The conversion of the operation

$$A \cdot [B(1 - e^{-B})^{-1} - 1]\mathfrak{D}_B C$$

utilizes the fact that C is a sum of commutators of various orders. Then, this operation must also yield such a form since the other terms of Eq. (4), $A\mathfrak{D}_A C$ and $A\mathfrak{D}_B C$, are such. Consider now the operation on the term $A \cdot B^2 A$ in C:

$$A \cdot [B(1 - e^{-B})^{-1} - 1]\ \mathfrak{D}_B A \cdot B^2 A = A \cdot \left\{A \cdot \left(\frac{B}{1 - e^{-B}} - 1\right)\right\}BA + A \cdot B\left\{A \cdot \left(\frac{B}{1 - e^{-B}} - 1\right)\right\}A, \qquad (7)$$

where the quantity in the curly brackets is to be taken as a single factor as regards the outermost dot. Clearly, these terms are not of the required form (thus the last term when written out is a difference of two *products* of commutators). However, they can be brought to the required form by suitable rearrangements. In fact the first term is

$$-\left\{A \cdot \left(\frac{B}{1 - e^{-B}} - 1\right)\right\} \cdot ABA,$$

and the second

$$-\left\{A\cdot\left(\frac{B}{1-e^{-B}}-1\right)\right\}\cdot ABA + \left\{A\cdot\left(\frac{B}{1-e^{-B}}-1\right)\right\}\cdot BAA$$

by the Jacobi identity $a\cdot bc + b\cdot ca + c\cdot ab = 0$. These are of the required form now. Effecting now the replacement $A \to \rho B$ results in

$$-\rho A\cdot\left(\frac{B}{1-e^{-B}}-1\right)B^2A$$

for the first term and in zero for the second term in (7). Both of these results can be generalized. In particular, we derive the rule that on the substitution $A \to \rho B$, the operation in question acting on an intermediate B yields zero. That this generalization is valid follows from writing $(A - \rho B)\cdot B$ instead of the $A\cdot B$ which stands at the head of all our commutators. Now we know that (on suitable rearrangement) the curly brackets will be brought into leading position and therefore $A - \rho B$ must come into some intermediate position in the commutator. The replacement $A \to \rho B$ will now clearly make all commutators vanish.

The same considerations show how to treat a term where the operation acts on B in the last position: only that commutator survives the rearrangement and the substitution in which $A - \rho B$ has got into the last position. The commutator is then *plus* or *minus* the original one with the curly brackets and $A - \rho B$ interchanged and the replacement $A \to \rho B$ effected in intermediate positions, the sign being positive (negative) for an odd (even) number of intermediate factors.

For the purpose of obtaining differential equations for F and G, one has to be unambiguous about the sign. To achieve this, one notes that the commutator terminating with $A - \rho B$ (i.e., that which yields the constant) is nonvanishing only when the total number of factors is odd (in other words, constant terms appear only in A, $A\cdot BA$, etc.) One also notes that the expression $B(1 - e^{-B})^{-1} - 1$ can be decomposed into an odd part $\frac{1}{2}B$, and an even part $B(1 - e^{-B})^{-1} - 1 - \frac{1}{2}B$. Combining these two facts one concludes that $\frac{1}{2}B$ will always appear with a changed sign, while the even part will maintain its sign. To summarize

$$A\cdot\left(\frac{B}{1-e^{-B}}-1\right)\mathfrak{D}_B C \to A\cdot\left(\frac{B}{1-e^{-B}}-1\right)$$

$$-\tfrac{1}{2}A\cdot\left(\frac{B}{1-e^{-B}}-1\right)A$$

$$-\rho A\cdot\left(\frac{B}{1-e^{-B}}-1\right)BF(B,\rho)B$$

$$+A\cdot\left(\frac{B}{1-e^{-B}}-1-\tfrac{1}{2}B\right)BF(B,\rho)(A-\rho B)$$

$$-\tfrac{1}{2}A\cdot B^2F(B,\rho)(A-\rho B)$$

$$-\rho A\cdot\left(\frac{B}{1-e^{-B}}-1\right)BG(B,\rho)A.$$

All the terms in Eq. (4) have now been converted into differential expressions. By equating separately those terms which end in B and those which end in A, we obtain the following coupled equations for F and G.

$$B(1+\rho)\frac{\partial}{\partial\rho}(B\rho F) - B^2\frac{\partial}{\partial B}(B\rho F) + 2B\left(\frac{B}{1-e^{-B}}-1-\tfrac{1}{2}B\right)(B\rho F) = \left(\frac{B}{1-e^{-B}}-1-\tfrac{1}{2}B\right).$$

$$(1+\rho)\frac{\partial}{\partial\rho}(B\rho^2G) - B\frac{\partial}{\partial B}(B\rho^2G) + \left(\frac{B}{1-e^{-B}}-2\right)B\rho^2G = \left[\frac{B}{1-e^{-B}}-B\right](B\rho F) - \tfrac{1}{2}\rho\left(\frac{B}{1-e^{-B}}-1\right).$$

The requirement, that F and G are power series of positive powers of B and ρ, determines the solutions uniquely. Thus, it turns out that we have not lost anything in the conversion $A \to \rho B$ or $C \to C'$.

By introducing the functions $\phi(B, \rho)$ and $\psi(B, \rho)$, we simplify the solutions substantially:

$$\phi(B,\rho) \equiv 1 + \tfrac{1}{2}B + B^2F(B,\rho) + \rho B^2G(B,\rho), \quad (8)$$

$$\psi(B,\rho) \equiv B^2G(B,\rho).$$

Then

$$C' = A + B + A\cdot\phi(B,\rho) + A\cdot BG[A - \rho B]. \quad (9)$$

The solutions of the differential equations can now be written as

$$\rho\phi(B,\rho) = (1+\rho)(1-e^{-\rho B})/(1-e^{-(1+\rho)B}) \quad (10)$$

$$\rho^2\psi(B,\rho) = \tfrac{1}{2} - \tfrac{1}{2}B\rho - \tfrac{1}{2}(1+\rho)\frac{e^{-\rho B}(1-e^{-B})}{1-e^{-(1+\rho)B}}\left[2 - \frac{1-e^{-B}}{1-e^{-(1+\rho)B}}\right] + \frac{1}{2B}(e^{B}-1) - \frac{1}{2B}\frac{e^{B}(1-e^{-B})^2}{1-e^{-B(1+\rho)}}. \quad (11)$$

In this paper, that part of ψ plays the main role which is even in the first argument. This is

$$\rho^2\psi_e(B,\rho) = -(1/2B) \times \{e^{-\rho B}(\bar{n}+1) + e^{\rho B}\bar{n} - (2\bar{n}+1)\} - \rho/2 + \tfrac{1}{2}(\rho^2/(1+\rho))\phi(B,\rho)\phi(-B,\rho). \quad (12)$$

with $\bar{n} = (e^{(\rho+1)B}-1)^{-1}$.

It can be verified that these solutions tally with the first few terms of C as given by Haussdorf [our Eq. (3)] and that F and G are of the required form.

6. HIGH-TEMPERATURE APPROXIMATION TO THE LINE SHAPE

We interrupt now the trend of the last section in order to show how we are going to use the results there found. We shall calculate the line shape for the cases I and II from the trace (1) by taking as the first approximation

$$C(\text{or } C') \sim A + B$$
$$= -\beta H_i + t\cdot(k/m)(\partial/\partial x_0) + it\cdot k^2/2m;$$
$$= -\beta H_i + itm\omega^2 a(x_{-1} - x_1) + itm\omega^2 a^2.$$

Let us "complete" the squares in the dynamical variables as follows

$$C = -\beta\{\cdots + (1/2m)(-i\,\partial/\partial x_0 - itk/\beta)^2 - \cdots + \tfrac{1}{2}m\omega^2(x_{-1}-x_0)^2 + \tfrac{1}{2}m\omega^2(x_0-x_1)^2 + \cdots\} + itk^2/2m - t^2k^2/2m\beta;$$
$$= -\beta\{\cdots - (1/2m)(\partial^2/\partial x_0^2) - \cdots + \tfrac{1}{2}m\omega^2(x_{-1} - x_0 - iat/\beta)^2 + \tfrac{1}{2}m\omega^2(x_0 - x_1 - iat/\beta)^2 + \cdots\} + itm\omega^2a^2 - t^2m\omega^2a^2/\beta.$$

The resultant expressions are apart from the constant terms, the Hamiltonians of a linear chain of simple harmonic oscillators with displaced equilibrium distances or momenta. Were these displacements real quantities, then the problem could be regarded, in the approximation considered, as solved: since the spectra of the "displaced" Hamiltonians are identical with the original ones, the traces in the numerator and denominator of (1) cancel exactly, *apart from the constant terms.*

But can the cancellation be achieved even for complex displacements? Yes, since a similarity transformation can bring the displaced Hamiltonians back to their original form and the trace is invariant under a similarity transformation. (We could argue alternatively from the fact that the complex Hamiltonian still has the same spectrum.) Now it is true that in general it is required that the transformation operator be unitary, which in our case it is not [for case I, it would be exp (tkx_0/β)]. However, the unitarity requirement is really too stringent, what is actually necessary is that the matrix of transformation between the new and original states should exist. When these states are those of harmonic oscillators, this is true.

The Fourier transform of the intensity is therefore Gaussian:

$$g(t) = \exp(itk^2/2m - t^2k^2/2m\beta)$$
$$g(t) = \exp(itm\omega^2a^2 - t^2m\omega^2a^2/\beta),$$

and so is the intensity distribution

$$I(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} g(t)e^{-iEt}\,dt$$
$$= (2\pi k^2/m\beta)^{-1/2}\exp - (E - k^2/2m)^2 m\beta/2k^2$$
$$= (4\pi m\omega^2a^2/\beta)^{-1/2}\exp - (E - m\omega^2a^2)^2\beta/4m\omega^2a^2.$$

Let us see now what are the conditions for the validity of the basic approximation of this section $C \sim A + B$, i.e., the neglect of the first and higher order commutators. We note that the expansion parameters in the series for C [see (1) and (3)] are $|\omega t|$ and $|\omega(it+\beta)|$, so that high temperatures, or more exactly $\omega\beta \ll 1$ is one condition. The second requirement $|\omega t| \ll 1$ is equivalent, after integration over t to $\beta\,|E - \bar{E}| \ll m\omega a^2$ and $\beta \ll ma^2$ for case II. That is, the validity of our approximation is guaranteed at sufficiently high temperatures and sufficiently near the center of the intensity curve.

An approximate solution for the displacement effect has already been obtained by Koide.[8] The result was a Gaussian curve with a mean of $m\sum(\Delta q_i)^2\omega_i^2$ and a square deviation of $m\sum(\Delta q_i)^2\omega_i^3(2\bar{n}_i+1)$. Δq is the displacement, ω the frequency, and $\bar{n}$ the mean occupation number of the mode: Since Koide followed the approach originated by Lamb, he expressed his results in terms of the normal modes (index j) of the lattice. The condition for this result is that $\beta \ll ma^2$ as above, without neces-

sarily $\omega\beta \ll 1$.[15] This is often realized in nature. If however, $w\beta \ll 1$, we regain our result, since

$$m \sum (\Delta q_i)^2 \omega_i^3 (2\bar{n}_i + 1) \simeq 2m/\beta \sum (\Delta q_i)^2 \cdot \omega_i^2.$$
$$= 4ma^2\omega^2/\beta.$$

The last two lines are equal as they give, in different representions, $2/\beta$ times the potential energy of the lattice in the final state at the instant when the atoms are at the equilibrium positions of the initial state. The equality is, of course, quite generally true in any dimensions. It may be said at this stage that the high-temperature expansion of the intensity comes out much simpler when obtained by the present dynamic method. In contrast, the normal mode approach which expresses the results in terms of unknown, or at best awkwardly determinable, parameters $(\Delta q, \omega)$ of the normal modes tends to obscure the physical meaning of the results.

Case I with the nuclear recoil differs from the one just discussed by writing k^2 instead of $2m^2\omega^2a^2$ in the condition for the expansion. There is however an additional situation which should be mentioned, where the lifetime of the excited state is short or comparable to the time of propagation of the disturbance to the neighboring lattice points. In this case also, the intensity distribution is Gaussian, as shown by Lamb,[4] and for high temperatures it is the same as for an ion gas. In fact, however, lifetimes are generally long (or not known). Thus Visscher[5] quotes $\sim 10^{-7}$ sec for gamma-ray capture in iridium. Optically excited states have natural lifetimes of about 10^{-11} sec, or about ten times longer than the time of propagation between lattice points.

7. GENERALIZATION OF THE FOREGOING

When one proceeds to include successively higher order commutators in C, one realizes that terms linear in the variables of successively more distant ions make their appearance. In fact, every second commutator pushes the disturbance one further step outward. In this way, we have the picture of the disturbance being propagated in time. We shall return to this picture later.

Suppose now that at a particular stage of approximation we have for C'

$$C' = -\beta H_i + \sum \alpha_i x_i + \sum \beta_i \frac{\partial}{\partial x_i} + \gamma(t, \beta),$$

where α_i, β_i (not to be confused with β) and the constant term $\gamma(t, \beta)$ will be found in the next section. We now complete the squares.

Write the Hamiltonian with the squares completed as

$$\cdots \tfrac{1}{2}m\omega^2 (x_{i-1} - x_i + a_{i-1} - a_i)^2 \cdots$$
$$- (\tfrac{1}{2}m)(\partial/\partial x_i + b_i)^2 - \cdots$$

and compare coefficients. Then

$$\alpha_i = -\beta m\omega^2(2a_i - a_{i-1} - a_{i+1})$$
$$\beta_i = (\beta/m)b_i.$$

We solve these equations in terms of the generating functions:

$$Q(r) = \sum \alpha_i r^i, \qquad P(r) = \sum \beta_i r^i. \tag{13}$$

The generating functions of a_i and b_i become, respectively,

$$\frac{1}{\beta m\omega^2} \frac{r}{(1-r)^2} Q(r) \quad \text{and} \quad \frac{m}{\beta} P(r).$$

From (1) we have now, since the traces cancel again

$$g(t) = \exp\{-(\beta/2m) \sum b_i^2 + \tfrac{1}{2}\beta m\omega^2 \times \sum (a_i - a_{i-1})^2 + \gamma(t, \beta)\}$$
$$= \exp\left\{-\frac{m}{2\beta} T_r{:} P(r)P\left(\frac{1}{r}\right) - \frac{1}{2\beta m\omega^2} T_r{:} \times \frac{r}{(1-r)^2} Q(r)Q\left(\frac{1}{r}\right) + \gamma(t, \beta)\right\}, \tag{14}$$

where $T_r{:}$ means "the term independent of r in the series expansion of : . . . ."

Note that, as long as only commutators up to a finite degree are considered in C, P and Q are polynominals in r and no questions of convergence arise. Ultimately, we shall, of course, consider the limiting cases of infinite chains and all the commutators in C.

8. THE GENERATING FUNCTIONS Q AND P

Consider the nth order commutators

$$A \cdot B^n = \sum (c_i^n x_i + d_i^n \partial/\partial x_i), \tag{15}$$

$$A \cdot B^{n-1}(A - \rho B) = e^n \qquad (n \geq 1), \tag{16}$$

$$A - \rho B = (c_i^0 x_i + d_i^0 \partial/\partial x_i) + e^0. \tag{17}$$

(n is a superscript and not a power on c, d, and e.) The coefficients c_i^0, d_i^0, and e^0 are determined by "initial conditions" from (5.I) and (5.II).

[15] The conditions $ma^2 \gg \beta$ and $\omega\beta \gtrsim 1$ imply that $t/\beta \sim |\rho| \ll 1$. In this case C is sufficiently approximated by terms linear in A, i.e., $C = A + B + A \cdot B/(1 - e^{-B})$, whence the formulation in terms of $\bar{n}$ can be obtained immediately.

$$A\cdot B^{n+1} = \sum (c_i^{n+1}x_i + d_i^{n+1}\,\partial/\partial x_i)$$
$$= A\cdot B^n B = \sum [c_i^n x_i\cdot B + d_i^n(\partial/\partial x_i)\cdot B]$$
$$= \sum\left[\frac{it}{\rho m}c_i^n\frac{\partial}{\partial \pi_i} + \frac{itm\omega^2}{\rho}d_i^n(2x_i - x_{i-1} - x_{i+1})\right],$$

where ρ was introduced in (5).

Equating coefficients, we obtain the recurrence relations

$$d_i^{n+1} = (it/\rho m)c_i^n,$$
$$c_i^{n+1} = (itm\omega^2/\rho)(2d_i^n - d_{i-1}^n - d_{i+1}^n) = (\rho m/it)\,d_i^{n+2}.$$

The last relation ressembles certain equations in problems of random walk. One usually solves these by means of generating functions. Let then

$$f(r,s) = \sum_{\substack{n=0\cdots\infty\\ i=-\infty\cdots\infty}} d_i^n r^i s^n,$$

and one finds that

$$f(r,s) = \frac{tk}{m}\left[1 - \frac{t^2\omega^2}{\rho^2}\frac{s^2(r-1)^2}{r}\right]^{-1} \qquad (18.\mathrm{I})$$
$$= \frac{t^2\omega^2 a}{\rho}\frac{(r - r^{-1})s}{1 - (t^2\omega^2/\rho^2)s^2(r-1)^2/r}, \qquad (18.\mathrm{II})$$

where the numerator has been determined by initial conditions. The generating function of c is $(m\rho/it)s^{-1}f(r,s)$. It is to be noted that terms linear in coordinates and in the momenta appear in alternate stages.

$$e^n = \sum_{i,k}\left[c_i^{n-1}x_i + d_i^{n-1}\frac{\partial}{\partial x_i}\,,\, c_k^0 x_k + d_k^0\frac{\partial}{\partial x_k}\right]$$
$$= \sum_i (c_i^0\,d_i^{n-1} - c_i^{n-1}\,d_i^0) \qquad (n \geq 1). \qquad (19)$$

As there are at most two nonzero c_i^0, d_i^0 the generating function of e^n may be written down very simply in terms of $f(r,s)$.

The generating functions $P(r)$, $Q(r)$ introduced in (13) give the coefficients of the dynamic variables in C', whereas the function $f(r,s)$ just found gives the coefficients in a *particular* commutator like $A\cdot B^n$. However, from Sec. 5, we know the coefficients of each $A\cdot B^n$ and $A\cdot B^{n-1}(A - \rho B)$ in C': these are the coefficients of z^n in $\phi(z,\rho)$ and $z^2G(z,\rho) = \psi(z,\rho)$ [see (8) and (9)].

We now have

$$Q(r) = m\rho/itT_s: s^{-1}\phi(s^{-1},\rho)f(r,s), \qquad (20)$$
$$P(r) = T_s: \phi(s^{-1},\rho)f(r,s), \qquad (21)$$

where the reader is reminded of the meaning of T_s in (14). The three terms occurring in the exponent of that expression can be written as

$$(-m/2\beta)T_{rsz}: f(r^{-1},z)f(r,s)\phi(z^{-1},\rho)\phi(s^{-1},\rho), \qquad (22)$$
$$\frac{m}{2\beta}\rho^2 T_{rsz}: \frac{1}{t^2\omega^2 sz}\frac{r}{(1-r)^2} \times f(r^{-1},z)f(r,s)\phi(z^{-1},\rho)\phi(s^{-1},\rho), \qquad (23)$$
$$e^0 + (m\rho/it)T_{rsz}: (s/z - 1)f(r^{-1},z)f(r,s)\psi(s^{-1},\rho). \qquad (24)$$

(The operator T_{rsz}: picks out the term independent of r, s, and z.)

These expressions represent the solution of the one-dimensional problem in general terms. In fact, the solution for three dimensions is very similar; what difference there is enters through f being the generating function of a three-dimensional random walk problem.

Further simplification results if one utilizes (18). Then, replacing the abstract operator T_r: by the contour integral $(2\pi i)^{-1}\int dr/r$ taken round a path encircling the origin that is wholly in the region of analyticity of the integrand, we can evaluate the integral and obtain for the case of nuclear recoil (case I)

$$\ln g(t) = -t^2(k/2m\beta)T_r:$$
$$\phi((t\omega/\rho)(r - r^{-1}),\rho)\phi((t\omega/\rho)(r^{-1} - r),\rho)$$
$$+ itk^2/2m\{1 + \rho T_r: [\psi((t\omega/\rho)(r - r^{-1}),\rho)$$
$$+ \psi((t\omega/\rho)(r^{-1} - r),\rho)]\}, \qquad (25.\mathrm{I})$$

where ϕ and ψ are given in (10) and (11). Likewise, in case II

$$\ln g(t) = -t^2(m\omega^2 a^2/2\beta)T_r:$$
$$(r + r^{-1})^2\phi((t\omega/\rho)(r - r^{-1}),\rho)\phi((t\omega/\rho)(r^{-1} - r),\rho)$$
$$+ itm\omega^2 a^2\{1 + \tfrac{1}{2}\rho T_r: (r + r^{-1})^2$$
$$\times [\psi((t\omega/\rho)(r - r^{-1}),\rho) + \psi((t\omega/\rho)(r^{-1} - r),\rho)]\}. \qquad (25.\mathrm{II})$$

9. THE ABSORPTION IN A MONATOMIC HARMONIC LATTICE

The results of Sec. 5, the functions ψ and ϕ, are left unchanged in three dimensions, since these depend only on the fact that H_f differs from H_i by, at most, a linear term. On the other hand, the completion of the squares and the random walk of Sec. 8, have to be redone for the Hamiltonian of the crystal. This Hamiltonian must be representable in the harmonic form if the approach of this paper is to

be applicable. This is the fundamental restriction on this work. (It should be noted that, in alternative methods, when one introduces normal modes, this restriction is implicitly also present.)

Let us write the harmonic Hamiltonian of a simple-cubic lattice (non-atomic) up to second-nearest neighbors[16])

$$\begin{aligned} H_i = \sum_{jkl}\Big\{ & -\frac{1}{2m}\frac{\partial^2}{\partial x_{jkl}^2} \\ & + \tfrac{1}{2}m\omega^2[(x_{jkl} - x_{j+1kl})^2 + \cdots] \\ & + \tfrac{1}{2}m\lambda^2[(x_{jkl} - x_{jk+1l})^2 + \cdots] \\ & + \tfrac{1}{2}m\nu^2[(x_{jkl} + x_{j+1k+1l})^2 + \cdots] \\ & + \tfrac{1}{2}m\mu^2[(x_{jkl} - x_{jk+1l+1})^2 + \cdots] \\ & + m\tau^2[(x_{jkl} - x_{j+1k+1l})(y_{jkl} - y_{j+1k+1l}) + \cdots]\Big\}. \end{aligned}$$

Only *types* of terms have been written down; what is not explicitly stated can be added by consideration of symmetry. For radial interactions, $\lambda = 0$, $\mu = 0$, $\nu = \tau$. In the following discussion we may assume a general three-dimensional disturbance for the ion labeled (000). The relation between H_i and H_f will be essentially the three-dimensional generalization of Eqs. (2).

As the first step we complete the squares in the expansion for C' (cf. Sec. 7), that is we find the relationship between the coefficients in the expression

$$\sum_{\substack{jkl \\ \xi=x,y,z}}\left[\alpha_{jkl}^{\xi}\xi_{jkl} + \beta_{jkl}^{\xi}\frac{\partial}{\partial\xi_{jkl}}\right], \tag{26}$$

on the one hand, and the constants of the (complex) displacements

$$\xi_{jkl} \to \xi_{jkl} + a_{jkl}^{\xi}, \qquad \partial/\partial\xi_{jkl} \to \partial/\partial\xi_{jkl} + b_{jkl}^{\xi},$$

on the other. In effect, we want to find the generating functions of a and b in terms of

$$\begin{aligned} P_\xi(p, q, r) \equiv P_\xi(\mathbf{p}) &= \sum \beta_{jkl}^{\xi}p^jq^kr^l, \\ Q_\xi(p, q, r) \equiv Q_\xi(\mathbf{p}) &= \sum \alpha_{jkl}^{\xi}p^jq^kr^l. \end{aligned}$$

($\xi = x, y, z$ is a superscript; j, k, l, are powers).

One finds immediately that $P_\xi^b(\mathbf{p}) = (m/\beta)P_\xi(\mathbf{p})$, but for the generating functions of a one derives a system of linear equations:

$$V_{(x,x)}Q_x^a + V_{(x,y)}Q_y^a + V_{(x,z)}Q_z^a = -1/\beta Q_x, \tag{27}$$

where explicitly

$$\begin{aligned} V_{(x,x)} = -m\{ & \omega^2(p-1)^2p^{-1} \\ & + \lambda^2[(q-1)^2q^{-1} + (r-1)^2r^{-1}] \\ & + \nu^2[(pq-1)^2p^{-1}q^{-1} + (pr-1)^2p^{-1}r^{-1} \\ & + (pq^{-1}-1)^2p^{-1}q + (pr^{-1}-1)^2p^{-1}r] \\ & + \mu^2[(qr-1)^2q^{-1}r^{-1} + (qr^{-1}-1)^2q^{-1}r]\} \\ V_{(x,y)} = -m\tau^2(pq + p^{-1}q^{-1} - pq^{-1} - p^{-1}q), \\ V_{(x,z)} = -m\tau^2(pr + p^{-1}r^{-1} - pr^{-1} - p^{-1}r), \end{aligned}$$

with two more equations obtained by cyclic interchanges of (x, y, z) and of (p, q, r). There is no point in writing out the solutions of (27) because we shall soon see that, similarly to the one dimensional problem, both Q and Q^a can be given explicitly in terms of $f_\xi(\mathbf{p}, s)$. This function, whose meaning is the obvious three-dimensional generalization of the work at the beginning of Sec. 8, is the fundamental, random-walk generating function of the problem. To find it we proceed as in that section and finish up with three equations of the type

$$\begin{aligned} & V_{(x,x)}f_x(\mathbf{p}, s) + V_{(x,y)}f_y(\mathbf{p}, s) + V_{(x,z)}f_z(\mathbf{p}, s) \\ & = -\frac{\rho^2 m}{t^2 s^2}\left[f_x(\mathbf{p}, s) - \underset{\text{I}}{f_x(\mathbf{p}, 0)} - s\underset{\text{II}}{\left(\frac{\partial}{\partial s}f_x(\mathbf{p}, s)\right)_{s=0}}\right] \end{aligned} \tag{28}$$

The time and temperature dependence enter through t and $\rho = -(1 - i\beta/t)^{-1}$. The solution of this set of inhomogeneous equations by means of matrix inversion is straightforward, in principle, and, when numbers are introduced, also in practice. There will be just one inhomogeneous term on the right-hand side in either of the situations I and II, as indicated.

There is also another, more abstract way of solving inhomogeneous equations, namely in terms of the eigensolutions of the corresponding homogeneous equations. This approach, which is computationally much more exacting, leads us to the normal-modes methods. We postpone its consideration to Sec. 11, where we show how our results can be reduced to the Lamb formula.

Next we have four equations

$$\begin{aligned} P_\xi(\mathbf{p}) &= T_s\colon f_\xi(\mathbf{p}, s)\phi(s^{-1}, \rho) \\ Q_\xi(\mathbf{p}) &= (m\rho/it)T_s\colon s^{-1}f_\xi(\mathbf{p}, s)\phi(s^{-1}, \rho) \\ P_\xi^b(\mathbf{p}) &= -m/\beta T_s\colon f_\xi(\mathbf{p}, s)\phi(s^{-1}, \rho) \\ Q_\xi^a(\mathbf{p}) &= (t/i\rho\beta)[T_s\colon sf_\xi(\mathbf{p}, s)\phi(s^{-1}, \rho) \\ & \qquad - (sf_\xi)_{s\to\infty}\phi(0, \rho)]. \end{aligned}$$

[16] C. Kittel, *Introduction to Solid State Physics* edited by F. Seitz and D. Turnbull (John Wiley & Sons, Inc., New York, 1959), 2nd ed.

The first two equations are, *mutatis mutandis*, Eqs. (21) and (20). The third has already been given. The last formula is the result of operating with T_s: $ts\phi(s^{-1}, \rho)/i\rho\beta$ on (28), comparing with (27), and deriving the asymptotic behavior of f from equation (28). The final result of this section achieves our goal, the intensity transform, with a compact formula

$$g(t) = \exp \sum_{\xi} \{T_{\mathbf{p}}: \tfrac{1}{2}[P^b_\xi(\mathbf{p})P_\xi(p^{-1}) - Q^a_\xi(\mathbf{p})Q_\xi(p^{-1})] + e^0 + m\rho/itT_{\mathbf{p}sz}: (sz^{-1} - 1)f_\xi(\mathbf{p}, z)f_\xi(p^{-1}, s)\psi(s^{-1}, \rho)\} \qquad (29)$$

$$p^{-1} = (p^{-1}, q^{-1}, r^{-1}).$$

This result contains the specialized universal (i.e., independent of the details of the harmonic lattice) Hausdorff functions ϕ and ψ, Eqs. (10) and (11); the random walk functions f of the lattice, the solution of Eqs. (28); and the number e^0, the constant part of $A - \rho B$. (It will be shown, however, in Sec. 11 that in most cases of interest the part containing ϕ cancels completely.) The operator $T_{\mathbf{p}sz}$: seeks out the term independent of all of the five variables $\mathbf{p}sz$. This means that the problem has been solved in terms of a five-dimensional integral, in which one integration can be performed trivially, and the solutions of a set of inhomogeneous equations whose coefficients are functions in a four-dimensional space.

We do not think that general remarks and vague advice on a computational program could add much to the value of this paper. More to the point will be our pending comparison with the normal mode approach. One should, nevertheless, point out that, apart from the obvious procedure of solving the inhomogeneous equations numerically and using the numbers immediately in the quadratures, there is also the possibility of a formal, algebraic solution coupled with the use of extensive tables of integrated generating functions.[17]

10. FURTHER GENERALIZATION

The notation for the monatomic simple-cubic lattice was purposefully chosen to be such, that only a few remarks should be necessary to deal with a general lattice, with many different atoms in the unit cell. The forces must be harmonic, however.

(j, k, l) will label the unit cell in a coordinate system appropriate to the lattice, ξ will run over $3s$ values for s atoms per unit cell. The form of the coefficients $V_{(\xi,\eta)}$ is indicated by the notation: you differentiate the potential with respect to ξ, you will then get terms containing the η of a particular unit cell. If this unit cell is (j', k', l'), with the cell of ξ regarded as the origin, then the coefficient of f_η in the analog of (28) will be got on replacing η by $p^j q^k r^l$. Further, the equation connecting P^a_ξ and P_ξ will be modified by using m_ξ instead of m.

Another interesting generalization of the previous work is when the radiating atom changes its equilibrium distance and receives a recoil at the same time. This may be realized if the crystal emits or captures a highly energetic charged particle, e.g., a heavy particle or a fast electron, or, less realistically, if an inner shell electron is transferred from one atom to its neighbors. (Here, however, a maximum recoil energy of only about 50 cm^{-1} seems possible.) In these events $f(s)$ has not got a definite parity and both odd and even parts of ψ enter in (29).

11. THE LAMB FORMULA. ASYMPTOTIC BEHAVIOR

We owe the reader the reduction of (29) to a sum over normal modes. As noted earlier, (28) can be solved for $\mathbf{f}(\mathbf{p}, s)$ in terms of the three eigenvectors $\mathbf{e}_i(\mathbf{p})$ and eigenvalues $s_i(\mathbf{p})$ of the homogeneous equation. In fact, when dealing with case I and a monatomic lattice,

$$\mathbf{f}(\mathbf{p}, s) = \sum_{i=1,2,3} \frac{\mathbf{e}_i(\mathbf{f}(\mathbf{p}, 0)\cdot\mathbf{e}_i)}{1 - s^2/s_i^2}.$$

When we substitute this expression into (29) and perform the operation T_{sz} [either by contour integration or by expansion of $(1 - s^2/s_i^2)^{-1}$ in a series], we find that the contribution from first line of (29) which involves ϕ cancels (by virtue of the orthonormal vectors $\mathbf{e}_i$) the contribution arising in (29) out of the third line of $\rho^2\psi_e$ in (12), while the $-\frac{1}{2}\rho$ suffices to cancel the constant $e^0 = itk^2/2m$, k being the recoil momentum. These remarkable cancellations will occupy us in more than one way. One needs to remember now that, although introduced in a different manner, the $\mathbf{e}_i(\mathbf{p})$ are in fact the polarizations of the $\mathbf{p}$th mode and that s_i are related to the eigenvalues of the mode by $s_i^{-1} = -it\omega_i/\rho$. Then from (29), (12) and with $\mathbf{k} = (k, 0, 0)$

$$\ln g(t) = T_{\mathbf{p}}: \sum_i \frac{(\mathbf{k}\cdot\mathbf{e}_i)^2}{2m\omega_i} \times [e^{i\omega_i t}(\bar{n} + 1) + e^{-i\omega_i t}\bar{n} - (2\bar{n} + 1)],$$

$$\bar{n} = (e^{\omega_i/kT} - 1)^{-1}.$$

The operator $T_{\mathbf{p}}$ can be transformed into a summation over normal modes by putting

[17] A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman, and H. W. Milnes, Mem. Acad. Roy. Belg. **14**, 7 (1960).

$$T_p: = (2\pi i)^{-1} \int dp/p: \qquad \text{(over the unit circle)},$$

and substituting $p = \lim_{L\to\infty} \exp 2\pi i l n/L$ (where l and L are the lengths of the unit cell and the lattice, respectively).

The intensity transform of the Franck-Condon case can also be reduced to a sum over normal modes. Two differences arise. One is that in terms of the fundamental constant a of the problem Δq_i (see Sec. 6) is given in a form which is more complicated than the case I counterpart. Secondly $T_s \to \int ds/s$ contains a nonvanishing contribution when taken over an infinite circle.

The fact that the net contribution to the intensity comes entirely from ψ is very suggestive. We have noted quite early that the successive order commutators in the Hausdorff function $C(A, B)$ denote the progressive outward propagation of the disturbance. ϕ and ψ differ in this respect, that the former consists of terms which denote a continual spreading of the disturbance, whereas in ψ the disturbance first spreads then reconverges at the source. This gives us a nice physical picture of how the radiating source puts out its feelers further and further, and regulates its emission according to what information it receives.

In this sense, then, the limit $t \to \infty$ corresponds to the accumulation, at the source, of information from the whole body of the crystal. However, from the point of view of emitted radiation, and if

$$\ln g(t) \to (\text{const})_1 \times t + (\text{const})_2 + O(1),$$

then an infinitely sharp line (eventually broadened by relaxation effects) will be received with a strength proportional to $\exp (\text{const})_2$.

The expansion of $\ln g(t)$ in the mentioned form can be carried out both for cases I and II for a three-dimensional crystal, when also $(\text{const})_1 = 0$. In two or one dimensions the expansion cannot be carried through, the trouble occurring at $\omega_i = 0$. Evidently the stability of the lattice is lacking in these cases.

$(\text{const})_2$ is the measure of the strength of the Mössbauer line in the nuclear-recoil case. It has been calculated by various elegant[5,6] methods, and also computed numerically as function of temperature. It will be noted, that it is directly given by our formulas on letting $e^{*\rho B} \to 0$ in (10) and (12). (This is required, since in the $\mathbf{p}$ integration, the exponential oscillates infinitely, when $t \to \infty$, giving a contribution $\propto t^{-1/2}$. Cf. the asymptotic behavior of the Bessel-function or of the integral treated in reference 17.)

For case II, one finds that

$$\ln g(t) \to \sum_\xi T_{p_s}:$$

$$\frac{im\rho}{t} [z f_\xi(\mathbf{p}, z)]_{z\to\infty} f_\xi(\mathbf{p}, s)(e^{(1+\rho)/s} - 1)^{-1},$$

a quantity which is actually independent of t.

12. CONCLUSION

In this paper, two problems in lattice dynamics have been approached from a new angle. The same approach should also be applicable to other problems: Primarily, we have in mind infrared absorption, quadrupole nuclear resonance, and radiation by an impurity in a lattice. In the course of our treatment an elaborate mathematical foundation had to be laid down and mastered. We must now ask ourselves, whether or not it was worthwhile.

As pointed out in the Introduction, we have presented solutions in a closed form and entirely within the framework (that is to say, using the data) of the problem posed. This must be regarded as the central achievement. Now, the normal modes' approach leads to a solution, which, in certain simplified situations but not in the general one, can be coupled with the data of the distribution of frequencies to yield numerical results. This is, therefore, a more practical, but not an entirely self-contained procedure. The question now arises: Can one not also determine the unknown parameters (ω_i, Δq_i, $\mathbf{k}\cdot\mathbf{e}_i$) of the normal modes' method *a priori*, from the data of the problem? Of course, one can, *in principle*, but for practical purposes this would require calculational efforts which are far in excess of the simple matrix inversions and quadratures of the present treatment. Alternatively, since the formulas of the normal modes' method are effectively diagonal sums, one could try to reduce these sums to others by formal methods not involving the diagonalization of the energy matrix, and would therefore be effectively equivalent to our result. In this connection we must reemphasize a shortcoming of our method which first introduces ϕ and the odd part of ψ, only to find later that both of these disappear in the final results. Now, we have shown at the end of Sec. 10 that there are problems in lattice dynamics where ψ enters and *stays*. We do not know whether this is ever so with ϕ, or whether there exists an equally general mathematical formalism which does without it.[18]

[18] It should be noted that in a recent work (R. Englman, "Solid-State and Molecular Theory Group," M.I.T. Quarterly Progress Report No. 42, April 15, 1962, unpublished) on the effect of a changed force constant on the spectral line, the function ϕ appears in the final result.

Statistical Thermodynamics of Nonuniform Fluids*

J. L. LEBOWITZ
Belfer Graduate School of Science, Yeshiva University, New York, New York
AND
J. K. PERCUS
Courant Institute of Mathematical Sciences, New York University, New York, New York
(Received 17 August 1962)

We have developed a general formalism for obtaining the low-order distribution functions $n_q(\mathbf{r}_1, \cdots, \mathbf{r}_q)$ and the thermodynamic parameters of nonuniform equilibrium systems where the nonuniformity is caused by a potential $U(\mathbf{r})$. Our method consists of transforming from an initial (uniform) density n_0 to the final desired density $n(\mathbf{r})$ via a functional Taylor expansion. When n_0 is chosen to be the density in the neighborhood of the r's we obtain n_q as an expansion in the gradients of the density. The expansion parameter is essentially the ratio of the microscopic correlation length to the scale of the inhomogeneities. Our analysis is most conveniently done in the the grand ensemble formalism where the corresponding thermodynamic potential serves as the generating functional [with $U(\mathbf{r})$ as the variable] for the n_q. The transition from $U(\mathbf{r})$ to $n(\mathbf{r})$ as the relevant variable is accomplished via the direct correlation function which enters very naturally, relating the change in U at $\mathbf{r}_2$ due to a change in n at $\mathbf{r}_1$. It is thus essentially the matrix inverse of the two-particle Ursell function. The recent results of Stillinger and Buff on the thermodynamic potentials for nonuniform systems follow as a special case of our analysis without any recourse to the virial expansion. Thus, they hold also in the liquid region. In a succeeding paper we apply our analysis to obtain the asymptotic behavior of the radial distribution function in a uniform system.

I. INTRODUCTION

IN a previous paper[1] we considered the form of the low-order distribution functions $n_q(\mathbf{r}_1, \cdots, \mathbf{r}_q)$ in a nonuniform system represented by a canonical ensemble. We investigated there both the case of an equilibrium system, where the nonuniformity comes from the existence of an external force field, and the case where the system is in a quasi-stationary nonequilibrium state characterized by local thermodynamic variables. In the latter situation the local equilibrium canonical ensemble represents only the lowest-order approximation to the true state of affairs. In either case our principal aim was to show that the low-order distribution functions n_q obtained from the N-particle canonical ensemble by integration over $N - q$ variables were local quantities, i.e., depended only on the density and temperature in the vicinity of the region where $\mathbf{r}_1, \cdots, \mathbf{r}_q$ are located. This is, of course, physically essential and intuitively "obvious."

We were able to prove this local property in reference 1 on the basis of a theorem (obtained rigorously only in the low-density limit) concerning the asymptotic form of the distribution n_{q+l} when the set of $q + l$ particles is separated into groups of q and l particles that are "far" apart,

$$n_{q+l} \to n_q n_l - \frac{1}{N^2}\frac{\partial N}{\partial \zeta}\left(\frac{N\,\partial n_q}{\partial N}\right)\left(\frac{N\,\partial n_l}{\partial N}\right), \qquad (1.1)$$

where ζ is the characteristic parameter of the particle reservoir, chemical potential divided by kT, which when placed in contact with our system, would yield $N(\zeta) = N$. Using (1.1), we were able to develop some general expressions for the changes of the n_q with variations in the thermodynamic parameters which showed that they depended only on the values of these parameters within a correlation length of n_q, i.e., the asymptotic N^{-1} part disappeared in the end result. More precisely, this is the region in which the Ursell function $\mathfrak{F}_q$ is different from zero for $N \to \infty$. We did not however carry out an explicit evaluation of these changes. This would indeed have been quite cumbersome within the canonical ensemble formalism, where N is fixed.

The purpose of this note is to carry out more explicitly, the evaluation of the n_q's and that of the thermodynamic properties of nonuniform equilibrium systems. This will enable us to make contact with other recent work on such systems,[2,3] and will also yield some new insights into the structure of fluids in general. For convenience, we shall use the

* Supported in part by the U. S. Air Force Office of Scientific Research, the United States Atomic Energy Commission and the National Aeronautic Space Agency.

[1] J. L. Lebowitz and J. K. Percus, Phys. Rev. **122**, 1675 (1961).

[2] F. H. Stillinger and F. P. Buff, J. Chem. Phys. **37**, 1 (1962).

[3] E. W. Hart, Phys. Rev. **113**, 412 (1959); **114**, 27 (1959); T. Hill, J. Chem. Phys. **30**, 1521 (1959); F. P. Buff and F. H. Stillinger, *ibid.* **25**, 312 (1956). See also T. Morita and K. Hiroike, Progr. Theoret. Phys. (Kyoto). **23**, 1003, (1960); C. De Dominicis, J. Math. Phys. **3**, 983 (1962).

grand ensemble formalism, where the existence of an infinite particle reservoir corresponds to making the N appearing in (1.1) effectively infinite and leads thus to true product distributions in the asymptotic region. The disappearance of the N^{-1} terms in (1.1) for an open system was proven rigorously in reference 1 in the region in which the virial expansion is valid.

II. GENERAL FORMALISM

The Hamiltonian of our system, when there are N particles present, will have the form

$$H_N = \sum_{i=1}^{N} p_i^2/2m + \sum_{i<j} \phi(\mathbf{r}_{ij}) + \sum_{i=1}^{N} U(\mathbf{r}_i), \qquad (2.1)$$

where $U(\mathbf{r})$ is the external potential. We can consider either the case where U determines the spatial extent of the system or that where the system is in a periodic box of volume $\Omega = L^3$, in which case U also has to be periodic. The grand-canonical phase-space ensemble density is given by

$$\rho_N(\mathbf{r}_1, \cdots, \mathbf{r}_N, \mathbf{p}_1, \cdots, \mathbf{p}_N) = (Z^{-1}/N!)e^{\beta\mu N - \beta H_N} = W(N)e^{-\beta H_N}/N!\, Q_N,$$

where

$$W(N) = e^{(\lambda+\beta\mu)N}Q_N/Z, \qquad Z = \sum_{N=0}^{\infty} Q_N e^{(\lambda+\beta\mu)N}, \qquad (2.2)$$

$$e^{(\lambda+\beta\mu)N}Q_N = \frac{1}{N!}\int \exp\left[\sum_{i=1}^{N}\gamma(\mathbf{r}_i) - \beta\sum_{i<i}\phi(\mathbf{r}_{ii})\right] d\mathbf{r}_1 \cdots d\mathbf{r}_N$$

and

$$\beta = (kT)^{-1}, \qquad \lambda = \tfrac{3}{2}\ln(2\pi mkT/h^2)$$
$$\gamma(\mathbf{r}) = \lambda + \beta\mu - \beta U(\mathbf{r}),$$

with T the temperature, μ the chemical potential, and Z the grand canonical partition function. In a uniform system (periodic boundaries, $U = 0$), $\ln Z$ reduces to $\beta p\Omega$ where p is the pressure, differing[4] from other definitions of the pressure (such as the average virial pressure $\beta\bar{p} = \partial \ln Z/\partial\Omega$) only by terms of order Ω^{-1}.

The lower order distribution functions f_q are defined as

$$f_q(\mathbf{r}_1, \cdots \mathbf{r}_q, \mathbf{p}_1, \cdots \mathbf{p}_q) = \sum_{N=0}^{\infty} W(N)\frac{N!}{(N-q)!}\int \rho_N\, d\mathbf{r}_{q+1}\cdots d\mathbf{r}_N\, d\mathbf{p}_{q+1}\cdots d\mathbf{p}_N$$
$$= \prod_{i=1}^{q}[(2\pi mkT)^{-3/2}e^{-\beta p_i^2/2m}]n_q(\mathbf{r}_1, \cdots, \mathbf{r}_q), \qquad (2.3)$$

where

$$n_q = \sum_N W(N)\frac{N!}{(N-q)!}\int \exp\left\{-\beta\sum_{i=1}^{N}\left[\sum_{i<i}\phi(\mathbf{r}_{ii}) + U(\mathbf{r}_i)\right]\right\}/N!\, Q_N\, d\mathbf{r}_{q+1}\cdots d\mathbf{r}_N$$
$$= \sum_N W(N)n_q(\mathbf{r}_1, \cdots, \mathbf{r}_q; N)$$
$$= \frac{1}{Z}\sum_N \frac{1}{(N-q)!}\int \exp\left\{\sum_{i=1}^{N}[\gamma(\mathbf{r}_i) - \beta\sum_{j<i}\phi(\mathbf{r}_{ij})]\right\} d\mathbf{r}_{q+1}\cdots d\mathbf{r}_N. \qquad (2.4)$$

Here $n_q(N)$ is the q-particle configurational distribution in a canonical ensemble of systems containing N particles each.

It is seen from (2.2) and (2.4) that $\ln Z$ may be used as a generating functional for the n_q's:

$$\delta \ln Z/\delta\gamma(\mathbf{r}_1) = n_1(\mathbf{r}_1) \equiv n(\mathbf{r}_1) \qquad (2.5)$$

$$\delta n(\mathbf{r}_1)/\delta\gamma(\mathbf{r}_2) = n_2(\mathbf{r}_1, \mathbf{r}_2) - n(\mathbf{r}_1)n(\mathbf{r}_2) + n(\mathbf{r}_1)\,\delta(\mathbf{r}_1 - \mathbf{r}_2) \qquad (2.6)$$

$$\delta n_q(\mathbf{r}_1, \cdots \mathbf{r}_q)/\delta\gamma(\mathbf{r}) = n_{q+1}(\mathbf{r}_1, \cdots \mathbf{r}_q, \mathbf{r}) + n_q(\mathbf{r}_1, \cdots, \mathbf{r}_q)\left[\sum_{i=1}^{q}\delta(\mathbf{r}_i - \mathbf{r}) - n(\mathbf{r})\right]. \qquad (2.7)$$

Some simplification of notation is achieved if we introduce the distribution functions $\hat{n}_q$ in which the various arguments are allowed to represent identical particles:

$$\hat{n}(\mathbf{r}) = n(\mathbf{r}), \quad \hat{n}_2(\mathbf{r}_1\mathbf{r}_2) = n_2(\mathbf{r}_1\mathbf{r}_2) + n(\mathbf{r}_1)\,\delta(\mathbf{r}_1 - \mathbf{r}_2),$$
$$\hat{n}_3(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) = n_3(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) + n_2(\mathbf{r}_1\mathbf{r}_2)\,\delta(\mathbf{r}_2 - \mathbf{r}_3) + n_2(\mathbf{r}_2\mathbf{r}_3)\,\delta(\mathbf{r}_3 - \mathbf{r}_1) + n_2(\mathbf{r}_3\mathbf{r}_1)\,\delta(\mathbf{r}_1 - \mathbf{r}_2) + n(\mathbf{r}_1)\,\delta(\mathbf{r}_1 - \mathbf{r}_2)\,\delta(\mathbf{r}_2 - \mathbf{r}_3), \cdots.$$

In terms of the $\hat{n}_q$'s, (2.7) assumes the form

$$\delta\hat{n}_q(\mathbf{r}_1, \cdots \mathbf{r}_q)/\delta\gamma(\mathbf{r}) = \hat{n}_{q+1}(\mathbf{r}_1, \cdots, \mathbf{r}_q, \mathbf{r}) - \hat{n}_q(\mathbf{r}_1, \cdots \mathbf{r}_q)n(\mathbf{r}). \qquad (2.8)$$

If we define the corresponding Ursell distributions

[4] J. L. Lebowitz and J. K. Percus, Phys. Rev. **124**, 1673 (1961).

$\hat{\mathfrak{F}}_q$ to be the same functions of the $\hat{n}_s$ as the $\mathfrak{F}_q$ are of the n_s:

$$\hat{\mathfrak{F}}_1(\mathbf{r}_1) = \hat{n}_1(\mathbf{r}_1), \hat{\mathfrak{F}}_2(\mathbf{r}_1\mathbf{r}_2) = \hat{n}_2(\mathbf{r}_1\mathbf{r}_2) - \hat{n}_1(\mathbf{r}_1)\hat{n}_1(\mathbf{r}_2), \cdots,$$

the sequence (2.8) finally reduces to

$$\delta\hat{\mathfrak{F}}_q(\mathbf{r}_1, \cdots \mathbf{r}_q)/\delta\gamma(\mathbf{r}) = \hat{\mathfrak{F}}_{q+1}(\mathbf{r}_1, \cdots \mathbf{r}_q, \mathbf{r}). \tag{2.9}$$

The matrix inverse of (2.6) will play an important role in what follows. Writing it in the form

$$[n(\mathbf{r}_1)n(\mathbf{r}_2)]^{1/2}\ \delta\gamma(\mathbf{r}_2)/\delta n(\mathbf{r}_1) = \delta(\mathbf{r}_1 - \mathbf{r}_2) - C(\mathbf{r}_2, \mathbf{r}_1), \tag{2.10}$$

we find from the defining interrelation

$$\int (\delta n(\mathbf{r}_2)/\delta\gamma(\mathbf{r}), [\delta\gamma(\mathbf{r})/\delta n(\mathbf{r}_1)]\, d\mathbf{r} = \delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{2.11}$$

that C satisfies the equation[5]

$$G(\mathbf{r}_2, \mathbf{r}_1) = C(\mathbf{r}_2, \mathbf{r}_1) + \int G(\mathbf{r}_2, \mathbf{r})C(\mathbf{r}, \mathbf{r}_1)\, d\mathbf{r}, \tag{2.12}$$

where

$$\begin{aligned} G(\mathbf{r}_2, \mathbf{r}_1) &= [n(\mathbf{r}_1)n(\mathbf{r}_2)]^{-1/2}\mathfrak{F}_2(\mathbf{r}_2, \mathbf{r}_1) \\ &= [n(\mathbf{r}_1)n(\mathbf{r}_2)]^{1/2}[g(\mathbf{r}_2\mathbf{r}_1) - 1] \qquad (2.13) \\ \mathfrak{F}_2(\mathbf{r}_1, \mathbf{r}_2) &= n_2(\mathbf{r}_1, \mathbf{r}_2) - n(\mathbf{r}_1)n(\mathbf{r}_2). \end{aligned}$$

The existence of the inverse (2.10) is a direct consequence of the use of a grand ensemble, for in a petit ensemble, $n(\mathbf{r})$ cannot be varied arbitrarily. It is clear from (2.12) that C is the generalization to nonuniform systems of the usual direct correlation function introduced by Ornstein and Zernike.[6] Equations (2.10) and (2.12) may also be written in the form

$$C(\mathbf{r}_1, \mathbf{r}_2) = \left(\frac{n(\mathbf{r}_1)}{n(\mathbf{r}_2)}\right)^{1/2} \frac{\delta \ln [n(\mathbf{r}_1)e^{-\gamma(\mathbf{r}_1)}]}{\delta \ln n(\mathbf{r}_2)}, \tag{2.14}$$

$$(1 - \mathbf{C}) = (1 + \mathbf{G})^{-1}, \tag{2.15}$$

the last being a matrix equation with $\mathbf{1}$ the unit matrix. The quantities G and C are always symmetric in their arguments; thus $\mathbf{G}$ and $\mathbf{C}$ are Hermitian.

III. LOCAL NATURE OF DISTRIBUTION FUNCTIONS

We shall now use the results of the previous section to examine the degree of locality of the distribution functions in a nonuniform system, independently of any assumption as to existence and rapidity of convergence of virial expansions. Our approach will be to start with a suitable uniform system and then, by altering the external potential, create the density pattern desired. The process of "turning on" an inhomogeneity in density then enables one to express parameters of a nonuniform system in terms of analogous quantities of a "nearby" uniform system. In fact, as we shall see, the omnipresence of the direct correlation function of microscopic range makes it possible to deal with very large inhomogeneities on a macroscopic level.

The effect of a finite density change $\Delta n(\mathbf{r})$ on a quantity f specified initially for $n_0(\mathbf{r})$ may be determined by a functional Taylor expansion about $f[n_0]$.[7] For this purpose, it is convenient to visualize the density change as due to a parameter α which varies from 0 to 1:

$$n(\mathbf{r}; \alpha) = \begin{cases} n_0(\mathbf{r}) & \text{at } \alpha = 0 \\ n(\mathbf{r}) & \text{at } \alpha = 1, \end{cases} \tag{3.1}$$

since an ordinary MacLaurin expansion, including remainder term, may then be used:

$$f[\alpha] = \sum_{j=0}^{s-1} \frac{1}{j!} \frac{\partial^j f(\alpha)}{\partial\alpha^j}\bigg|_{\alpha=0} + \int_0^1 \frac{\partial^s f(\alpha)}{\partial\alpha^s} \frac{(1-\alpha)^{s-1}}{(s-1)!}\, d\alpha. \tag{3.2}$$

Now employing the chain rule

$$\frac{\partial}{\partial\alpha} = \int \frac{\partial n(\mathbf{r}; \alpha)}{\partial\alpha} \frac{\delta}{\delta n(\mathbf{r}; \alpha)}\, d\mathbf{r}, \tag{3.3}$$

we have the desired functional expansion

$$\begin{aligned} f[n] = f[n_0] &+ \int \frac{\partial n(\mathbf{r}_1; \alpha)}{\partial\alpha}\bigg|_0 \frac{\delta f[n_0]}{\delta n_0(\mathbf{r}_1)}\, d\mathbf{r}_1 \\ &+ \frac{1}{2}\left[\iint \frac{\partial n(\mathbf{r}_1; \alpha)}{\partial\alpha} \frac{\partial n(\mathbf{r}_2; \alpha)}{\partial\alpha}\bigg|_0 \right. \\ &\times \frac{\delta^2 f[n_0]}{\delta n_0(\mathbf{r}_1)\ \delta n_0(\mathbf{r}_2)}\, d\mathbf{r}_1\, d\mathbf{r}_2 \\ &\left. + \int \frac{\partial^2 n(\mathbf{r}_1; \alpha)}{\partial\alpha^2}\bigg|_0 \frac{\delta f[n_0]}{\delta n_0(\mathbf{r}_1)}\, d\mathbf{r}_1\right] \\ &+ \cdots + \int_0^1 \frac{(1-\alpha)^{s-1}}{(s-1)!}\left[\int \cdots \int \frac{\partial n(\mathbf{r}_1; \alpha)}{\partial\alpha} \cdots \right. \\ &\times \frac{\partial n(\mathbf{r}_s; \alpha)}{\partial\alpha} \frac{\delta^s f[n(\alpha)]}{\delta n(\mathbf{r}_1; \alpha) \cdots \delta n(\mathbf{r}_s; \alpha)}\, d\mathbf{r}_1 \cdots d\mathbf{r}_s \\ &\left. + \cdots + \int \frac{\partial^s n(\mathbf{r}_1; \alpha)}{\partial\alpha^s} \frac{\delta f[n(\alpha)]}{\delta n(\mathbf{r}_1; \alpha)}\, d\mathbf{r}_1\right] d\alpha. \end{aligned} \tag{3.4}$$

In the special case in which we choose, as we may,

$$\begin{aligned} n(\mathbf{r}; \alpha) &= (1 - \alpha)n_0(\mathbf{r}) + \alpha n(\mathbf{r}) \\ &= n_0(\mathbf{r}) + \alpha\, \Delta n(\mathbf{r}), \end{aligned} \tag{3.5}$$

[5] J. Yvon, Suppl. Nuovo cimento 9, 144 (1958); J. K. Percus, Phys. Rev. Letters 8, 462 (1962).

[6] L. S. Ornstein and F. Zernike, Proc. Acad. Sci. Amsterdam 17, 793 (1914).

[7] A systematic examination of the use of functional differentiation to obtain general results applicable to nonuniform systems has been made by G. Stell (to be published).

Eq. (3.4) reduces to

$$f[n] = \sum_{i=0}^{s-1} \frac{1}{j!} \int \cdots \int \Delta n(\mathbf{r}_1) \cdots \Delta n(\mathbf{r}_i) \times \frac{\delta^i f[n_0]}{\delta n_0(\mathbf{r}_1) \cdots \delta n(\mathbf{r}_i)} d\mathbf{r}_1 \cdots d\mathbf{r}_i + \int_0^1 \frac{(1-\alpha)^{s-1}}{(s-1)!} \int \cdots \int \Delta n(\mathbf{r}_1) \cdots n(\mathbf{r}_s) \times \frac{\delta^s f[n(\alpha)]}{\delta n(\mathbf{r}_1;\alpha) \cdots \delta n(\mathbf{r}_s;\alpha)} d\mathbf{r}_1 \cdots d\mathbf{r}_s d\alpha. \quad (3.6)$$

It is to be noted that the variational derivatives which have direct significance are [see (2.5)–(2.7)] with respect to $\gamma(\mathbf{r})$, not $n(\mathbf{r})$. We must then transform appropriately:

$$\frac{\delta f[n]}{\delta n(\mathbf{r})} = \int \frac{\delta f[n]}{\delta \gamma(\mathbf{r}')} \frac{\delta \gamma(\mathbf{r}')}{\delta n(\mathbf{r})} d\mathbf{r}',$$

$$\frac{\delta^2 f[n]}{\delta n(\mathbf{r}_1)\, \delta n(\mathbf{r}_2)} = \iint \frac{\delta^2 f[n]}{\delta \gamma(\mathbf{r}_1')\, \delta \gamma(\mathbf{r}_2')} \frac{\delta \gamma(\mathbf{r}_1')}{\delta n(\mathbf{r}_1)} \frac{\delta \gamma(\mathbf{r}_2')}{\delta n(\mathbf{r}_2)} d\mathbf{r}_1' \, d\mathbf{r}_2' + \int \frac{\delta f[n]}{\delta \gamma(\mathbf{r}')} \frac{\delta^2 \gamma(\mathbf{r}')}{\delta n(\mathbf{r}_1)\, \delta n(\mathbf{r}_2)} d\mathbf{r}', \cdots . \quad (3.7)$$

The successive derivatives of γ are obtained from the general matrix relation

$$D(A^{-1})_{ij} = -\sum (A^{-1})_{ik}\, D(A_{kl})(A^{-1})_{lj} \quad (3.8)$$

for an arbitrary first-order differential operator D. Thus,

$$\frac{\delta^2 \gamma(\mathbf{r}')}{\delta n(\mathbf{r}_1)\, \delta n(\mathbf{r}_2)} = \int \left(\frac{\delta \gamma(\mathbf{r}'')}{\delta n(\mathbf{r}_2)}\right) \frac{\delta}{\delta \gamma(\mathbf{r}'')} \left(\frac{\delta n}{\delta \gamma}\right)^{-1} (\mathbf{r}', \mathbf{r}_1)\, d\mathbf{r}'' \quad (3.9)$$

becomes

$$\frac{\delta^2 \gamma(\mathbf{r}')}{\delta n(\mathbf{r}_1)\, \delta n(\mathbf{r}_2)} = -\int \frac{\delta \gamma(\mathbf{r}'')}{\delta n(\mathbf{r}_2)} \frac{\delta \gamma(\mathbf{r}')}{\delta n(\mathbf{r}_1')} \times \frac{\delta^2 n(\mathbf{r}_1')}{\delta \gamma(\mathbf{r}'')\, \delta \gamma(\mathbf{r}''')} \frac{\delta \gamma(\mathbf{r}''')}{\delta n(\mathbf{r}_1)} d\mathbf{r}_1' \, d\mathbf{r}'' \, d\mathbf{r}''', \quad (3.10)$$

and higher derivatives are similarly found.

We may term a distribution function $n_s(\mathbf{x}_1 \cdots \mathbf{x}_s)$ in an inhomogeneous system local in character if its deviation from the value it would have in a uniform system, of density $n(\mathbf{x})$ with $\mathbf{x}$ in the region $\mathbf{x}_1, \cdots, \mathbf{x}_s$, is of the order of a molecular dimension divided by the scale of the inhomogeneity. Let us suppose for definiteness that, having fixed the point $\mathbf{x}$, then throughout the system

$$|n(\mathbf{r}) - n(\mathbf{x})| \leq [|\mathbf{r} - \mathbf{x}|/L(\mathbf{x})]n(\mathbf{x}). \quad (3.11)$$

If $f[n] = n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n)$, then Eq. (3.6), by virtue of (2.7), (3.7), and (2.8), reduces for the case when (3.6) is truncated after one term,

$$n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n) = n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n(\mathbf{x})) + \int_0^1 \iint \Delta n(\mathbf{r}) \Big\{ n_{s+1}(\mathbf{x}_1, \cdots \mathbf{x}_s, \mathbf{r}'; n(\alpha)) + n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n(\alpha)) \Big[\sum_1^s \delta(\mathbf{x}_i - \mathbf{r}') - n(\mathbf{r}') \Big] \Big\} \times [n(\mathbf{r})n(\mathbf{r}')]^{-1/2} [\delta(\mathbf{r} - \mathbf{r}') - C(\mathbf{r}, \mathbf{r}'; n(\alpha))]\, d\mathbf{r}'\, d\mathbf{r}\, d\alpha. \quad (3.12)$$

Assuming that

$$\int [n(\mathbf{r})n(\mathbf{r}')]^{-1/2} \, |C(\mathbf{r}, \mathbf{r}'; n(\alpha))| \, d\mathbf{r} \leq (K_1 - 1)/n(\mathbf{r}', \alpha),$$

$$\int [n(\mathbf{r})n(\mathbf{r}')]^{-1/2} \, |\mathbf{r} - \mathbf{r}'| \, |C(\mathbf{r}, \mathbf{r}'; n(\alpha))| \, d\mathbf{r}/K_1 \leq \lambda_1/n(\mathbf{r}', \alpha),$$

$$\int \left| \frac{n_{s+1}(\mathbf{x}_1, \cdots \mathbf{x}_s, \mathbf{r}'; n(\alpha))}{n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n(\alpha))n(\mathbf{r}'; \alpha)} - 1 \right| d\mathbf{r}' \leq (K_2 - s)/n(\mathbf{x}),$$

$$\int |\mathbf{r}' - \mathbf{x}| \left| \frac{n_{s+1}(\mathbf{x}_1, \cdots \mathbf{x}_s; \mathbf{r}'; n(\alpha))}{n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n(\alpha))n(\mathbf{r}\ ; \alpha)} - 1 \right| d\mathbf{r}'/K_2 \leq \lambda_2 n(\mathbf{x}) \quad (3.13)$$

exist over the full integration range, it follows from $|\Delta n(\mathbf{r})| \leq [n(\mathbf{x})/L(\mathbf{x})](|\mathbf{r}' - \mathbf{x}| + |\mathbf{r} - \mathbf{r}'|)$ and (3.13) that

$$|n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n) - n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n(\mathbf{x}))| \leq \left(K_1 K_2 \frac{\lambda_1 + \lambda_2}{L(x)} + s K_1 \frac{R}{L(\mathbf{x})} \right) \times \int n_s(\mathbf{x}_1, \cdots \mathbf{x}_s; n(\alpha))\, d\alpha, \quad (3.14)$$

where $\mathbf{x}$ is the point of smallest density in the set $\mathbf{x}_1, \cdots \mathbf{x}_s$ and R is the diameter of the set.

Thus n_s will certainly exhibit local character in the sense described above if $C(\ ,\ \mathbf{r})$ and $n_{s+1}(\ ,\ \mathbf{r})/n_s(\ )n(\mathbf{r}) - 1$ fall off faster than $1/r^4$ as $r \to \infty$. By including further terms in (3.6), one can similarly produce a remainder term which is bounded by a higher power of a microscopic to macroscopic length. Disregarding the remainder, let us investigate the form of these terms, which are expressible in terms of parameters of a uniform system. If we apply (3.7) and (3.10) to (3.6), and

make use of (2.9), the full Taylor expansion of $f[n]$ becomes

$$
\begin{aligned}
f[n] &= f[n_0] + \int \frac{\delta f(n_0)}{\delta\gamma(\mathbf{r}')} [n_0(\mathbf{r})n_0(\mathbf{r}')]^{-1/2} \\
&\times [\delta(\mathbf{r}-\mathbf{r}') - C_0(\mathbf{r},\mathbf{r}')]\, \Delta n(\mathbf{r})\, d\mathbf{r}\, d\mathbf{r}' \\
&+ \frac{1}{2}\int \frac{\delta^2 f(n_0)}{\delta\gamma(\mathbf{r}_1')\,\delta\gamma(\mathbf{r}_2')} [n_0(\mathbf{r}_1)n_0(\mathbf{r}_1') \\
&\times n_0(\mathbf{r}_2)n_0(\mathbf{r}_2')]^{-1/2}[\delta(\mathbf{r}_1-\mathbf{r}_1') - C_0(\mathbf{r}_1,\mathbf{r}_1')] \\
&\times [\delta(\mathbf{r}_2-\mathbf{r}_2') - C_0(\mathbf{r}_2,\mathbf{r}_2')] \\
&\times \Delta n(\mathbf{r}_1)\, \Delta n(\mathbf{r}_2)\, d\mathbf{r}_1'\, d\mathbf{r}_2'\, d\mathbf{r}_1\, d\mathbf{r}_2 \\
&- \frac{1}{2}\int \frac{\delta f(n_0)}{\delta\gamma(\mathbf{r}')} \hat{\mathfrak{F}}_{30}(\mathbf{r}_1'\mathbf{r}''\mathbf{r}''')[n_0(\mathbf{r}_2)n_0(\mathbf{r}'') \\
&\times n_0(\mathbf{r}_1')n_0(\mathbf{r}')n_0(\mathbf{r}_1)n_0(\mathbf{r}''')]^{-1/2} \\
&\times [\delta(\mathbf{r}_2-\mathbf{r}'') - C_0(\mathbf{r}_2,\mathbf{r}'')][\delta(\mathbf{r}_1'-\mathbf{r}') \\
&- C_0(\mathbf{r}_1',\mathbf{r}')][\delta(\mathbf{r}_1-\mathbf{r}''') - C_0(\mathbf{r}_1,\mathbf{r}''')] \\
&\times \Delta n(\mathbf{r}_1)\, \Delta n(\mathbf{r}_2)\, d\mathbf{r}_1'\, d\mathbf{r}'\, d\mathbf{r}''\, d\mathbf{r}'''\, d\mathbf{r}_1\, d\mathbf{r}_2 + \cdots . \qquad (3.15)
\end{aligned}
$$

This is in essence a local decomposition. That is, $\delta^s f/\delta\gamma(\mathbf{r}_1)\cdots\delta\gamma(\mathbf{r}_s)$ will, in general, vanish unless $\mathbf{r}_1, \cdots, \mathbf{r}_s$ are within a microscopic correlation range of each other, and of any space points associated with f itself. The $\hat{\mathfrak{F}}_s$ likewise vanish asymptotically with respect to all arguments. The connecting links are always direct correlation factors $C_0(r, r')$, and since these are similarly short range (indeed the range of the internal potential, according to the P.Y. approximation[8]), the various Δn are thereby restricted to the same region. In fact, since each Δn is restricted to a predetermined region, one can absorb large spacial inhomogeneities and still utilize a Taylor expansion

$$
\begin{aligned}
\Delta n(\mathbf{r}) &= \Delta n(\mathbf{x}) + (\mathbf{r}-\mathbf{x})\cdot\nabla(\Delta n(\mathbf{x})) \\
&+ \tfrac{1}{2}(\mathbf{r}-\mathbf{x})(\mathbf{r}-\mathbf{x}):\nabla\nabla(\Delta n(\mathbf{x})) + \cdots \qquad (3.16)
\end{aligned}
$$

Consider once more the distribution functions and in particular the s-body Ursell distribution $\hat{\mathfrak{F}}_s(\mathbf{x}_1, \cdots \mathbf{x}_s)$, in an inhomogeneous system. We shall again compare this to the corresponding distribution for a uniform system at constant density $n_0(\mathbf{x}) = n(\mathbf{x})$ for some point $\mathbf{x}$ in the vicinity of $\mathbf{x}_1, \cdots, \mathbf{x}_s$, which we will later choose more carefully. Now $\Delta n(\mathbf{r}) = n(\mathbf{r}) - n(\mathbf{x})$ and (3.16) becomes

$$
\begin{aligned}
\Delta n(\mathbf{r}) &= (\mathbf{r}-\mathbf{x})\cdot\nabla n(\mathbf{x}) \\
&+ \tfrac{1}{2}(\mathbf{r}-\mathbf{x})(\mathbf{r}-\mathbf{x}):\nabla\nabla n(\mathbf{x}) + \cdots . \qquad (3.17)
\end{aligned}
$$

Furthermore, for isotropic potentials, the "unperturbed" distributions are functions of interparticle distance alone. Hence

$$
\begin{aligned}
&\int [\delta(\mathbf{r}-\mathbf{r}') - C_0(\mathbf{r},\mathbf{r}')](\mathbf{r}-\mathbf{x})\, d\mathbf{r} \\
&\quad = \int [\delta(\mathbf{r}) - C_0(\mathbf{r})](\mathbf{r}+\mathbf{r}'-\mathbf{x})\, d\mathbf{r} \\
&\quad = (\mathbf{r}'-\mathbf{x})\int [\delta(\mathbf{r}) - C_0(\mathbf{r})]\, d\mathbf{r} \\
&\quad = -(\mathbf{x}-\mathbf{r}')\beta/n_0\chi_0 \qquad (3.18)
\end{aligned}
$$

where χ is the isothermal compressibility [see Eq. (4.17)]. In a similar fashion

$$
\begin{aligned}
&\int [\delta(\mathbf{r}-\mathbf{r}') - C_0(\mathbf{r},\mathbf{r}')](\mathbf{r}-\mathbf{x})(\mathbf{r}-\mathbf{x})\, d\mathbf{r} \\
&\qquad = (\mathbf{x}-\mathbf{r}')(\mathbf{x}-\mathbf{r}')\beta/n_0\chi_0 - \tfrac{1}{3}(\Lambda^2\beta/n_0\chi_0)\mathbf{1}
\end{aligned}
$$

where

$$
\begin{aligned}
\Lambda^2 &= \int r^2 C_0(\mathbf{r})\, d\mathbf{r} \Big/ \int [\delta(\mathbf{r}) - C_0(\mathbf{r})]\, d\mathbf{r} \\
&= \frac{\int r^2 G_0(\mathbf{r})\, d\mathbf{r}}{\int [\delta(\mathbf{r}) + G_0(\mathbf{r})]\, d\mathbf{r}} \qquad (3.19)
\end{aligned}
$$

Combining (3.15)–(3.19), we obtain in general

$$
\begin{aligned}
f[n(r)] &= f_0[n(x)] \\
&+ \frac{\beta}{n_0^2\chi_0}\int \frac{\delta f_0}{\delta\gamma(\mathbf{r}')} \{[-(\mathbf{x}-\mathbf{r}')\cdot\nabla n(\mathbf{x})] \\
&+ \tfrac{1}{2}[(\mathbf{x}-\mathbf{r}')(\mathbf{x}-\mathbf{r}') - \tfrac{1}{3}\Lambda^2\mathbf{1}]\cdot\nabla\nabla n(\mathbf{x})\}\, d\mathbf{r}' \\
&+ \frac{1}{2}\left(\frac{\beta}{n_0^2\chi_0}\right)^2 \iint \frac{\delta^2 f_0}{\delta\gamma(\mathbf{r}_1')\,\delta\gamma(\mathbf{r}_2')} \\
&\times (\mathbf{x}-\mathbf{r}_1')(\mathbf{x}-\mathbf{r}_2')\, d\mathbf{r}_1'\, d\mathbf{r}_2' : \nabla n(\mathbf{x})\, \nabla n(\mathbf{x}) \\
&- \frac{1}{2}\frac{\beta^2}{n_0^3\chi_0^2}\iint \frac{\delta f_0}{\delta\gamma(\mathbf{r}')} \hat{\mathfrak{F}}_{30}(\mathbf{r}_1'\mathbf{r}_2'\mathbf{r}_3') \\
&\times [\delta(\mathbf{r}_1') - C_0(\mathbf{r}_1')](\mathbf{x}-\mathbf{r}'-\mathbf{r}_2') \\
&\times (\mathbf{x}-\mathbf{r}'-\mathbf{r}_3')\, d\mathbf{r}' \cdots d\mathbf{r}_3 : \nabla n(\mathbf{x})\, \nabla n(\mathbf{x}) + \cdots , \qquad (3.20)
\end{aligned}
$$

where throughout subscript zero indicates that the quantities are those for a uniform system at density $n(\mathbf{x})$. According to (2.9), the modified Ursell distributions are readily amenable to expansion in locally uniform parameters. We have from (3.20),

[8] J. K. Percus and J. G. Yevick, Phys. Rev. 110, 1 (1958); referred to as P. Y.; J. Lebowitz, J. Percus and I. Zucker have shown recently that for a one dimensional gas of hard spheres $C(r)$ vanishes outside the hard sphere diameter (to be published). G. Stell has shown that $C(r) = 0$ outside the hard sphere diameter implies the P. Y. equation for any dimension (to be published).

choosing $\mathbf{x} = \sum_1^s \mathbf{x}_i/s$ and observing the structure of the "unperturbed" distributions

$$\hat{\mathfrak{F}}_2(\mathbf{x}_1, \mathbf{x}_2) = \hat{\mathfrak{F}}_{20}(\mathbf{x}_1, \mathbf{x}_2)$$
$$+ \left\{ \frac{1}{2}\left(\frac{\beta}{n_0\chi_0}\right) \int \hat{\mathfrak{F}}_{30}(\mathbf{x}_1\mathbf{x}_2, \mathbf{r}') \right.$$
$$\times [(\mathbf{x} - \mathbf{r}')(\mathbf{x} - \mathbf{r}') + \tfrac{1}{3}\Lambda^2 1]\, d\mathbf{r}' : \nabla\nabla n(\mathbf{x})$$
$$+ \frac{1}{2}\left(\frac{\beta}{n_0\chi_0}\right)^2 \int \hat{\mathfrak{F}}_{40}(\mathbf{x}_1\mathbf{x}_2\mathbf{r}_1\mathbf{r}_2)(\mathbf{x} - \mathbf{r}_1)$$
$$\times (\mathbf{x} - \mathbf{r}_2)\, d\mathbf{r}_1\, d\mathbf{r}_2 : \nabla n(\mathbf{x})\, \nabla n(\mathbf{x})$$
$$- \frac{1}{2}\left(\frac{\beta}{n_0\chi_0}\right)^2 \int \hat{\mathfrak{F}}_{30}(\mathbf{x}_1\mathbf{x}_2\mathbf{r})$$
$$\times \hat{\mathfrak{F}}_{30}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)[\delta(\mathbf{r}_1) - C_0(\mathbf{r}_1)](\mathbf{x} - \mathbf{r}_1)(\mathbf{x} - \mathbf{r})$$
$$\left. \times d\mathbf{r} \cdots d\mathbf{r}_3 : \nabla n(\mathbf{x})\, \nabla n(\mathbf{x}) + \cdots \right\}, n_0 \qquad (3.21)$$

while $\hat{\mathfrak{F}}_s$, for $s > 2$, contains a first-order term as well.

IV. THERMODYNAMIC POTENTIALS

We can also use the results of Sec. II to obtain explicit expressions for the various thermodynamic potentials in nonuniform systems. The expressions are generalizations of those found by Stillinger and Buff.[2] For comparison of notation, the quantity

$$X(\mathbf{r}_1, \mathbf{r}_2) \equiv C(\mathbf{r}_1, \mathbf{r}_2)/[n(\mathbf{r}_1)n(\mathbf{r}_2)]^{1/2}, \qquad (4.1)$$

of Stillinger and Buff, will be employed.

Let us recall the interrelations between the commonly used potentials in a grand canonical ensemble. By virtue of its role as generating function, the grand canonical potential

$$\Xi = \frac{1}{\beta} \ln Z \qquad (4.2)$$

is basic to our considerations. A generalized Legendre transformation with respect to $\gamma(\mathbf{r})$ suffices to introduce the remaining potentials. From (2.5), coupled with the expression $G = N\mu = \int \mu n(\mathbf{r})\, d\mathbf{r}$ for the Gibbs free energy, we have

$$\int \gamma(\mathbf{r})\, \delta\Xi/\delta\gamma(\mathbf{r})\, d\mathbf{r} = G - \int U(\mathbf{r})n(\mathbf{r})\, d\mathbf{r} + \lambda N/\beta. \qquad (4.3)$$

The Helmholtz free energy $F = G - \Xi$ then results from

$$\int \gamma(\mathbf{r})\, \delta\Xi/\delta\gamma(\mathbf{r})\, d\mathbf{r} - \Xi = F - \int U(\mathbf{r})n(\mathbf{r})\, d\mathbf{r} + \lambda N/\beta. \qquad (4.4)$$

It is of course a consequence of (4.4) that

$$[\delta/\delta n(\mathbf{r})]\left[F - \int U(\mathbf{r})n(\mathbf{r})\, d\mathbf{r} + \lambda N/\beta \right] = \gamma(\mathbf{r})/\beta \qquad (4.5)$$

so that F too serves as a generating function.

Now we would like to demonstrate the local nature of the thermodynamic potentials, i.e., the extent to which local energy densities can be defined in an inhomogeneous system. Let us first consider Ξ, and integrate the infinitesimal change under a density variation, $\delta\Xi = \int [\delta\Xi/\delta n(\mathbf{r})]\, \delta n(\mathbf{r})\, d\mathbf{r}$, to obtain the $s = 1$ case of (3.4), with (3.7) applied,

$$\Xi[n] = \Xi[n_0] + \int_0^1 \iint \frac{\partial n(\mathbf{r}; \alpha)}{\partial\alpha} \frac{\delta\Xi[n(\alpha)]}{\delta\gamma(\mathbf{r}'; \alpha)} \frac{\delta\gamma(\mathbf{r}'; \alpha)}{\delta n(\mathbf{r}; \alpha)}\, d\mathbf{r}\, d\mathbf{r}'\, d\alpha. \qquad (4.6)$$

From (2.5) and (2.10) with (4.1), it follows that

$$\beta\Xi[n] = \beta\Xi[n_0] + (N - N_0) - \int_0^1 \iint n(\mathbf{r}'; \alpha) \frac{\partial n(\mathbf{r}; \alpha)}{\partial\alpha} X(\mathbf{r}\mathbf{r}'; \alpha)\, d\mathbf{r}\, d\mathbf{r}'\, d\alpha. \qquad (4.7)$$

In particular, if the density is turned on from $n_0 = 0$, in which case $\beta\Xi[n_0] = N_0$, we may write

$$\beta\Xi = \int \left[n(\mathbf{r}) - \int_0^1 \int n(\mathbf{r}; \alpha) \frac{\partial n(\mathbf{r}'; \alpha)}{\partial\alpha} \times X(\mathbf{r}\mathbf{r}'; \alpha)\, d\mathbf{r}'\, d\alpha \right] d\mathbf{r} = \int \hat{p}(\mathbf{r})\, d\mathbf{r}. \qquad (4.8)$$

Here $\hat{p}(r)$ is a fictitious pressure which coincides with the thermodynamic pressure in a uniform system (which has been turned on uniformly). Clearly however, $\hat{p}(\mathbf{r})$ as here defined depends upon the exact process, represented by α, which has been used to get from $n_0 = 0$ to $n(\mathbf{r})$. In the special case $n(\mathbf{r}; \alpha) = \alpha n(\mathbf{r})$, Eq. (4.8) becomes identical with Eq. (25) of Stillinger and Buff. If $X(\mathbf{r}\mathbf{r}'; \alpha)$ remains short range throughout the transformation from n_0 to $n(\mathbf{r})$, then $\hat{p}(\mathbf{r})$ depends only upon $n(\mathbf{r}')$ in the vicinity of $\mathbf{r}' = \mathbf{r}$ and thus $\hat{p}(\mathbf{r})$ is a valid energy density; this may prohibit thermodynamic transitions during the "turning on" and hence restrict the locality property to gases.

Equations (26) and (27) of Stillinger and Buff, which express the Gibbs and Helmholtz free energies as volume integrals involving X, may be derived in a similar fashion. In Eq. (4.3), we have already made use of the fact that, from $\beta G = \int n(\mathbf{r})\, \beta\mu\, d\mathbf{r}$, one has

$$\beta G = \int n(\mathbf{r})\gamma(\mathbf{r})\, d\mathbf{r} + \int [\beta U(\mathbf{r}) - \lambda]n(\mathbf{r})\, d\mathbf{r}. \qquad (4.9)$$

To obtain the form of (4.8), $\gamma(\mathbf{r})$ is then expanded as well. It is only necessary to observe that $n_0 = 0$ may be achieved by increasing the external potential without bound so that all particles are squeezed back into the reservoir. Then, it is easy to see, from (2.4), that $\gamma(\mathbf{r}) - \ln n(\mathbf{r})$ approaches zero. Hence, precisely in the fashion of (4.6) to (4.8), we find

$$\gamma(\mathbf{r}) - \ln n(\mathbf{r}) = -\int_0^1 \int \frac{\partial n(\mathbf{r}';\alpha)}{\partial \alpha} X(\mathbf{r}\mathbf{r}',\alpha)\, d\mathbf{r}'\, d\alpha \qquad (4.10)$$

or

$$\beta G = \int n(\mathbf{r})[\beta U(\mathbf{r}) + \ln n(\mathbf{r}) - \lambda] - \int_0^1 \int n(\mathbf{r}) \frac{\partial n(\mathbf{r}';\alpha)}{\partial \alpha} X(\mathbf{r}\mathbf{r}';\alpha)\, d\mathbf{r}'\, d\alpha\, d\mathbf{r}. \qquad (4.11)$$

From $F = G - \Xi$, then

$$\beta F = \int \Big\{ n(\mathbf{r})[\beta U(\mathbf{r}) + \ln n(\mathbf{r}) - \lambda] - \int_0^1 \int (n(\mathbf{r}) - n(\mathbf{r};\alpha)) \frac{\partial n(\mathbf{r}';\alpha)}{\partial \alpha} \times X(\mathbf{r}\mathbf{r}';\alpha)\, d\mathbf{r}'\, d\alpha \Big\} d\mathbf{r}. \qquad (4.12)$$

The specialization $n(\mathbf{r};\alpha) = \alpha n(\mathbf{r})$ again recovers the results of Stillinger and Buff.

One would now like to expand the presumably local energy densities in terms of the local particle density and its derivatives, as in (3.21). The lack of uniqueness suggests conceptual difficulties, and this is reinforced by the fact that in expanding a total energy, there is no "neighborhood" uniform density from which one can develop the actual density. However, the expression (4.9) is itself a unique decomposition of the Gibbs free energy, with energy density

$$n(\mathbf{r})\mu = \beta^{-1}[n(\mathbf{r})\gamma(\mathbf{r}) + n(\mathbf{r})(\beta U(\mathbf{r}) - \lambda)]. \qquad (4.13)$$

If $\gamma(\mathbf{r})$ is then expanded according to (3.20) about its value at uniform density $n(\mathbf{r})$, we readily obtain

$$\beta\mu = \beta U(\mathbf{r}) + \beta\mu_0[n(\mathbf{r})] - \tfrac{1}{6}(\Lambda^2\beta/n^2\chi_0)\nabla^2 n(\mathbf{r}) - \tfrac{1}{6} l^2(\beta/n^2\chi_0)^2[\nabla \cdot n(\mathbf{r})^2] + \cdots, \qquad (4.14)$$

where Λ^2 has been defined in Eq. (3.19) and

$$l^2 = n \int \hat{\mathfrak{F}}_{30}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)[\delta(\mathbf{r}_1) - C_0(\mathbf{r}_1)]\mathbf{r}_2 \cdot \mathbf{r}_3\, d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3. \qquad (4.15)$$

The quantities with subscript zero refer, as in Sec. III, to uniform systems at density $n(\mathbf{r})$, and thus Λ^2 and l^2 are also functions of $n(\mathbf{r})$. Equation (4.15), which defines the Gibbs free energy per particle in a nonuniform system as a "local functional" of the particle density, differs from the other free energy density expressions of this section in that it does not depend explicitly on the "path" along which $n(\mathbf{r})$ has been built up. We have tried to find similar path independent expressions for the other free energy densities but have not succeeded so far.

Equation (4.15) may also be thought of as determining the density $n(\mathbf{r})$ for a system with a chemical potential μ, which is a constant independent of $\mathbf{r}$, subject to an external field $U(\mathbf{r})$. When the external field causes only slight inhomogeneities in the fluid, the gradient terms may be neglected to obtain

$$\mu \approx U(\mathbf{r}) + \mu_0(n(\mathbf{r})). \qquad (4.16)$$

This equation will have a unique solution for $\mu(\mathbf{r})$, which may be but slightly inhomogeneous, only when one is not near a phase transition. Equation (4.16) will also be valid generally for a dilute gas where $\mu_0(n) \propto \ln n$, since the remaining terms in (4.14) vanish as $n \to 0$.

Finally, we shall make some remarks concerning another thermodynamic parameter, the isothermal compressibility. For a uniform system, with a constant change δn due to a constant change $\delta\gamma$, we have

$$\delta\Xi = \delta n \int [\delta\Xi/\delta\gamma(\mathbf{r})][\delta\gamma(\mathbf{r})/\delta n(\mathbf{r}')]\, d\mathbf{r}\, d\mathbf{r}',$$

yielding, as in (4.7),

$$\partial(\beta p\Omega)/\partial n = \Omega - n \int X(\mathbf{r} - \mathbf{r}')\, d\mathbf{r}\, d\mathbf{r}',$$

so that

$$\chi_0^{-1} = n\, \partial p/\partial n = nkT\Big[1 - n \int X(\mathbf{r})\, d\mathbf{r}\Big]. \qquad (4.17)$$

By virtue of the relation

$$\int [g(\mathbf{r}) - 1]\, d\mathbf{r} = \Big[\int X(\mathbf{r})\, d\mathbf{r}\Big]\Big\{1 + n \int [g(\mathbf{r}) - 1]\, d\mathbf{r}\Big\}, \qquad (4.18)$$

where

$$g(\mathbf{r}_1 - \mathbf{r}_2) = n_2(\mathbf{r}_1, \mathbf{r}_2)/n^2,$$

obtained by integrating Eq. (2.13), (4.17) is identical with the well-known Ornstein-Zernike compressibility expression. Equation (4.18) is a special case of a simple important relationship in uniform systems. Since G and C then depend only upon the difference of their arguments, they are diagonal in

Fourier transform space k, so that (2.12) implies

$$C(\mathbf{k}) = G(\mathbf{k})/[1 + G(\mathbf{k})]. \tag{4.19}$$

Analogous relations for nonuniform systems may be obtained by multiplying (2.12) by $[n(\mathbf{r}_1)n(\mathbf{r}_2)]^{1/2}$ and integrating with respect to $\mathbf{r}_2$:

$$\begin{aligned}\int \mathfrak{F}_2(\mathbf{r}_1, \mathbf{r}_2)\, d\mathbf{r}_2 &= \int C(\mathbf{r}_1, \mathbf{r}_2)[n(\mathbf{r}_1)n(\mathbf{r}_2)]^{1/2} \\ &\quad \times \left[1 + n^{-1}(\mathbf{r}_2) \int \mathfrak{F}_2(\mathbf{r}_2, \mathbf{r})\, d\mathbf{r}\right] d\mathbf{r}_2 \\ &= n(\mathbf{r}_1) \int X(\mathbf{r}_1, \mathbf{r}_2)\Big[n(\mathbf{r}_2) \\ &\quad + \int \mathfrak{F}_2(\mathbf{r}_2, \mathbf{r})\, d\mathbf{r}\Big] d\mathbf{r}_2. \end{aligned} \tag{4.20}$$

Now it follows from the definition of n_q, (2.4), that

$$\begin{aligned}&\int [n_{q+1}(\mathbf{r}_1, \cdots \mathbf{r}_{q+1}) - n_q(\mathbf{r}_1, \cdots \mathbf{r}_q)n(\mathbf{r}_{q+1})]\, d\mathbf{r}_{q+1} \\ &= \sum W(N)[Nn_q(N) - \langle N\rangle n_q(N)] - qn_q \\ &= kT\, \partial n_q/\partial\mu - qn_q. \end{aligned} \tag{4.21}$$

In particular, therefore,

$$\int \mathfrak{F}_2(\mathbf{r}_1, \mathbf{r}_2)\, d\mathbf{r}_2 = kT\, \partial n(\mathbf{r}_1)/\partial\mu - n(\mathbf{r}_1). \tag{4.22}$$

Combining (4.22) and (4.20) yields

$$\frac{\partial n(\mathbf{r}_1)}{\partial\beta\mu} = n(\mathbf{r}_1)\left\{1 + \int X(\mathbf{r}_1, \mathbf{r}_2)\, \frac{\partial n(\mathbf{r}_2)}{\partial\beta\mu}\, d\mathbf{r}_2\right\}. \tag{4.23}$$

Equation (4.23) reduces to (4.17) for a uniform system when use is made of the relation

$$dp/dn = nd\mu/dn. \tag{4.24}$$

V. CONCLUSION

The general formalism developed here, which is summarized in Eq. (3.15), is suitable for application to many specific problems. We have used (3.15)[9] with $f[n] = \gamma(\mathbf{r})$ and an external potential $U(\mathbf{r})$ caused by keeping one of the fluid molecules fixed at the origin to investigate the asymptotic form of $g(r)$ in a uniform system. This is compared with the Ornstein-Zernike results obtainable from a truncation of (4.14). We also plan to apply our formalism to obtain an expression for the surface tension. This will be related to finding 'path independent' expressions for the other free energy densities (besides the Gibbs). The latter would also yield an expression for the entropy density which might be of use also for nonequilibrium systems.

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Perpendicular Susceptibility of the Ising Model

MICHAEL E. FISHER
Wheatstone Physics Laboratory, King's College, London W. C. 2, England
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A high-temperature expansion of the partition function for a lattice of N spins with Hamiltonian

$$\mathcal{H} = -J \sum_{(ij)} \sigma_i^z \sigma_j^z - mH_z \sum_i \sigma_i^z - mH_x \sum_i \sigma_i^x$$

is derived and thence an expansion for the zero-field perpendicular susceptibility is found. By perturbation theory, $\chi_\perp(T)$ is also expanded at low temperatures and seen, in general, to increase with T from the value $\chi_\perp(0) = Nm^2/q\,|\,J\,|$, where q is the coordination number of the lattice. The perpendicular susceptibility is re-expressed in terms of near neighbor pair and higher-order spin correlation functions in zero field. This yields *exact closed formulas* for the linear chain, the Bethe pseudolattices, and for the plane square and honeycomb lattices. The behavior of $\chi_\perp(T)$ in the critical region is investigated for these lattices and for the plane superexchange lattice.

1. INTRODUCTION

THE Ising model, originally proposed as a model of ferromagnetism,[1] is one of the simplest examples of a many-body system in statistical mechanics. In spite of its simplicity, however, it embodies the essential features underlying the cooperative behavior of many physical systems such as antiferromagnets, binary alloys, and condensing gases. Its study has proved valuable theoretically in elucidating the behavior of more complex models and the rigorous results obtained by Onsager,[2] Kaufman,[3,4] Yang,[5] and others[6] for two-dimensional Ising lattices have thrown considerable light on the deficiencies of approximate statistical methods. Most approximations have been misleading guides to the true behavior in the transition region which, from a fundamental viewpoint, is one of the most interesting aspects of the problem.

Although the Ising model of a spin system is frequently regarded as a semi-classical model, the spin variables s_i commuting with one another and taking only the definite values ± 1, it may be regarded equally well as a fully quantum mechanical model with extreme anisotropic exchange coupling between spins. In terms of the Pauli spin operators σ_i^x, σ_i^y, and σ_i^z the Hamiltonian for a lattice of N spins may then be written

$$\mathcal{H} = -J \sum_{(ij)} \sigma_i^z \sigma_j^z - mH_z \sum_i \sigma_i^z - mH_x \sum_i \sigma_i^x, \tag{1.1}$$

where the z axis is the axis of anisotropy and where H_z and H_x are the parallel and perpendicular components of the external magnetic field. The exchange energy J is positive for a ferromagnet and, in spectroscopic notation, $m = \frac{1}{2}g\beta$. The first sum is over all pairs of interacting spins (nearest neighbors on the lattice) and the following sums run over all spins.

The zero-field *parallel* susceptibility $\chi_\parallel(T)$ corresponding to the Hamiltonian (1.1) has been the subject of quite intensive study, mainly based on series expansions,[7-11] but the *perpendicular* susceptibility $\chi_\perp(T)$ seems not to have been investigated.

In this paper we show first how the zero-field perpendicular susceptibility may be expanded both at high and at low temperatures. By using a general method for calculating the effects of perturbations on Ising models, we then relate $\chi_\perp(T)$ to the zero-field spin-spin correlations of the types $\langle \sigma_i^z \sigma_j^z \rangle = \langle s_i s_j \rangle$, $\langle \sigma_i^z \sigma_j^z \sigma_k^z \sigma_l^z \rangle = \langle s_i s_j s_k s_l \rangle$, etc. Our most interesting results follow from this relation, since by utilizing the work of Kaufman and Onsager,[4] it leads to exact closed formulas for the perpendicular susceptibility of various one- and two-dimensional lattices. For the lattices that have a transition, the precise behavior of $\chi_\perp(T)$ in the critical region is thus revealed. It may be summarized generally by saying that $\partial\chi_\perp/\partial T$ displays a singularity similar to the specific heat anomaly but of relatively smaller amplitude.[8,9]

The high- and low-temperature expansions are

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discussed in Secs. 2 and 3, respectively, while the general relation with the correlation functions is expounded in Sec. 4. Detailed results for individual lattices are obtained and examined in Sec. 5. Some of the leading results of the paper were announced without proof in an earlier paper[12] where they were discussed briefly in relation to the more general anisotropic Heisenberg Hamiltonian and to approximate treatments of antiferromagnetism.

2. HIGH-TEMPERATURE EXPANSIONS

The partition function for a lattice of N spins is

$$Z_N(T) = \mathrm{Tr}^N\{\exp(-\mathcal{H}/kT)\} \tag{2.1}$$

where Tr^N denotes the trace taken in the 2^N-dimensional space of the spin operators for all sites. It is convenient to introduce the dimensionless temperature and field variables

$$K = J/kT \tag{2.2}$$

and

$$L_x = mH_x/kT, \qquad L_z = mH_z/kT. \tag{2.3}$$

A high-temperature expansion of the partition function is obtained in the normal way by expanding the exponential in (2.1) and taking the trace term by term which yields

$$Z_N(T) = \sum_{r=0}^{\infty} \mathrm{Tr}^N\{(-\mathcal{H}/kT)^r\}/r!. \tag{2.4}$$

On expanding $(-\mathcal{H}/kT)^r$ by the binomial theorem [where $\mathcal{H}$ is given by (1.1)] we obtain products of the spin operators σ_i^x and σ_i^z in all permutations. The trace of any odd power of σ_i^x or σ_i^z vanishes and since $\sigma_i^x\sigma_i^z = i\sigma_i^y$, all products vanish unless *both* σ_i^x and σ_i^z appear to even powers. This shows, as expected, that only even powers of H_x and H_z appear in the expansions. The absolute value of a nonvanishing product containing a given set of σ_i^x and σ_i^z, corresponding to a selection of "bonds," "z spins," and "x spins" from the Hamiltonian is the same for all possible permutations of the operators. In virtue of the commutation relation $\sigma_i^x\sigma_i^z = -\sigma_i^z\sigma_i^x$, however, the *sign* depends on the number of permutations needed to gather together all the σ_i^x factors for each site. In expanding the partition function we require the *mean value* of a product averaged over all possible permutations. Since operators on different sites commute, the mean values may be calculated by multiplying the absolute value by a factor ν_i for each site. The factor ν_i can depend only on the number of x operators, say $2p_i$, and the number of z operators, say $2q_i$, which appear in the product and must be independent of the number of operators for other sites.

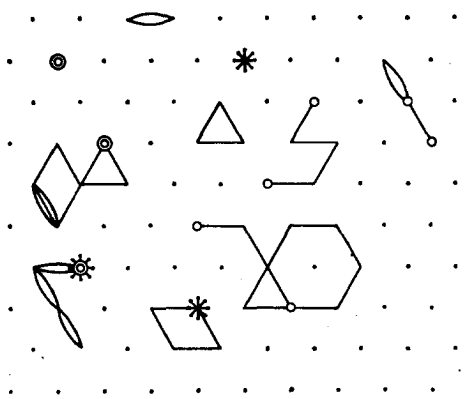

FIG. 1. A high-order graph entering the general expansion of the partition function at high temperatures. Each circle denotes a z spin and the stars denote doubled x spins.

The foregoing arguments show that the partition function in an arbitrary field may be expanded in terms of graphs constructed according to the following rules:

(a) A graph consists of n bonds between lattice sites and s x spins and t z spins on lattice sites;

(b) *Repeated bonds* are allowed, that is, between a given pair of sites k there may be m_k bonds where $\sum m_k = n$;

(c) At each site i there must be $p_i = 0, 1, 2, 3, \cdots$ *doubled* x spins, where $\sum 2p_i = s$;

(d) At each site i there must also be $u_i = 0, 1, 2, \cdots$ single z spins where $\sum u_i = t$;

(e) The number of bonds v_i meeting at the site i must be such that $u_i + v_i$ is even and equal to $2q_i$.

A typical high-order graph exhibiting some of the possibilities is shown in Fig. 1.

If $G_N(n, s, t)$ is the number of graphs of a given type G on the lattice of N sites, which satisfy the rules (a) to (e), the partition function is given by

$$Z_N(K, L_x, L_z) = 2^N \sum_G G_N(n, s, t) K^n L_x^s L_z^t \prod_k (1/m_k!) \times \prod_i \nu(p_i, q_i)/(2p_i)!\, u_i!, \tag{2.5}$$

where the explicit expression for the factors $\nu(p, q)$ is given in Eq. (2.11) below. If the lattice is considered wrapped on a torus and graphs looping the torus are neglected, $G_N(n, s, t)$ is a polynomial in N. If we denote the coefficient of N in this polynomial by $g_1(n, s, t)$, then the free energy per spin in the

[12] M. E. Fisher, Physica **26**, 618 (1960).

limit N is simply[13]

$$-F/kT = \ln 2 + \sum_G g_1(n, s, t)K^n L_x^s L_z^t \prod_k (1/m_k!) \times \prod_i \nu(p_i, q_i)/(2p_i)!u_i!, \quad (2.6)$$

from which series for the thermodynamic and magnetic properties can be deduced by differentiation in the standard manner. For the perpendicular susceptibility in zero field we evidently need consider only closed graphs consisting of a single doubled x spin and n bonds of which an even number meet at each vertex (site).

To complete the analysis we must calculate the vertex function $\nu(p, q)$, which takes account of the commutation rules at a site where both x and z operators are present. (If either p or q vanishes, then clearly $\nu = 1$.) To accomplish this we introduce the generating function

$$\psi(\xi, \zeta) = \mathrm{Tr}\,\{\exp(\xi\sigma^x + \zeta\sigma^z)\}. \quad (2.7)$$

On expanding the exponential and using the definition of $\nu(p, q)$, we have

$$\psi(\xi, \zeta) = 2\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\nu(p, q)\xi^{2p}\zeta^{2q}/(2p)!(2q)!. \quad (2.8)$$

On the other hand we have generally

$$\mathrm{Tr}\,\{\exp \mathbf{A}\} = \exp\lambda_1 + \exp\lambda_2, \quad (2.9)$$

where λ_1 and λ_2 are the eigenvalues of the 2×2 matrix $\mathbf{A}$. Diagonalizing the operator $\xi\sigma^x + \zeta\sigma^z$ yields $\lambda = \pm(\xi^2 + \zeta^2)^{1/2}$ so that

$$\psi(\xi, \zeta) = 2\cosh(\xi^2 + \zeta^2)^{1/2}. \quad (2.10)$$

Expanding the right-hand side of this expression in powers of ξ and ζ and comparing with (2.8) yields

$$\nu(p, q) = \binom{p+q}{p}\Big/\binom{2p+2q}{2p}. \quad (2.11)$$

This is symmetric in p and q as it should be and reduces correctly to unity if p or q vanishes. For the perpendicular susceptibility in zero field we need only

$$\nu(1, q) = 1/(2q + 1). \quad (2.12)$$

Using the above theory, the high temperature expansion for the perpendicular susceptibility in zero field for a general lattice is found to be

$$\chi_\perp(T) = (Nm^2/kT)\{1 - \tfrac{1}{3}qK^2 - 2p_3K^3 - [\tfrac{8}{5}p_4 - \tfrac{1}{15}q(q+1)]K^4 + \cdots\}. \quad (2.13)$$

In this expression q is the coordination number of the lattice and p_3 and p_4 are the number of triangles and squares per site of the lattice as defined and tabulated by Domb and Sykes.[13,14] For lattices like the plane square and simple cubic where all polygons have an even number of sides, it can be generally seen from the expansion (2.5) that $\chi_\perp$ is an even function of K and hence is the same for antiferromagnetic as for ferromagnetic coupling. The magnetic anisotropy is similarly found to be

$$\chi_\perp - \chi_\parallel = -qJNm^2(kT)^{-2}\{1 + (q - \tfrac{2}{3})K + [q^2 - 2q + \tfrac{2}{3} - 4(p_3/q)]K^2 + [(q-1)^3 - \tfrac{11}{15}q + \tfrac{3}{5} - 12(q-1)(p_3/q) - \tfrac{16}{3}(p_4/q)]K^3 + \cdots\}. \quad (2.14)$$

(Note that J is negative for an antiferromagnet). The anisotropy predicted by this formula is much greater than observed in most real materials. This is indicative of the extreme anisotropy of the pure Ising coupling.[15]

3. LOW-TEMPERATURE EXPANSIONS

Low-temperature expansions for the *parallel* susceptibility are readily derived[13] by expanding the partition function in powers of $z = e^{-2K}$ and $\mu = e^{-2L}$. The leading term as $T \to 0$ for a lattice which orders at $T = 0$ is

$$\chi_\parallel(T) = (4Nm^2/kT)\exp(-2q\,|J|/kT), \quad (T \to 0). \quad (3.1)$$

To calculate the *perpendicular* susceptibility we set $H_x = 0$ in (1.1) and treat the perpendicular term $\mathcal{H}_\perp = -mH_x\sum\sigma_i^x$ as a perturbation to the Ising coupling $\mathcal{H}_0 = -J\sum\sigma_i^z\sigma_j^z$. The states $|n\rangle$ and energy levels E_n of $\mathcal{H}_0$ are discrete and may be classified by assigning definite values of σ_i^z at each site ('up' and 'down' spins). In a field the energy levels change and the partition function may written

$$Z_N = \sum_n \exp[-E_n(H_x)/kT]. \quad (3.2)$$

Using the notation

$$\langle A_n\rangle = Z_N^{-1}\sum_n A_n\exp(-E_n/kT) \quad (3.3)$$

for the canonical average of a state variable, the perpendicular susceptibility is

$$\chi_\perp(T) = -\langle\partial^2 E_n/\partial H_x^2\rangle + (1/kT)\langle(\partial E_n/\partial H_x)^2\rangle - (1/kT)\langle\partial E_n/\partial H_x\rangle^2. \quad (3.4)$$

[13] C. Domb, Advance in Phys. 9, 220, 283, 296 (1960).

[14] C. Domb and M. F. Sykes, Phil. Mag. 2, 733 (1957).

[15] If the transverse coupling terms $-\gamma J\sum(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y)$ are added to the Hamiltonian (1.1), the leading term in Eq. (2.14) is multiplied by $(1 - \gamma)$ so that all anisotropy vanishes for Heisenberg coupling ($\gamma = 1$).

In zero-field, the derivatives of the energy levels are given by the standard perturbation formulas

$$-\partial E_n/\partial H_x = m(n \mid \sum_i \sigma_i^x \mid n) \tag{3.5}$$

and

$$-\frac{1}{2}\frac{\partial^2 E_n}{\partial H_x^2} = m^2 \sum_{n'} \frac{(n \mid \sum \sigma_i^x \mid n')^2}{E_{n'} - E_n} \tag{3.6}$$

provided that degeneracy can be neglected. The matrix elements of $\sum \sigma_i^x$ between any two states of the same S^z (total z component of spin) vanish since the operator σ_i^x merely inverts the spin on the site i. Thus, if there is no degeneracy between states of *different* S^z, the first derivatives $\partial E_n/\partial H_x$ vanish identically and only the first term of (3.4) need be retained.

A low-temperature expansion for a lattice that orders at $T = 0$ may then be derived by considering the states in order of increasing energy above the ground state and using (3.3) and (3.6). [Actually it is only necessary to consider the terms proportional to N in the numerator of (3.3).] The calculations are quite straightforward. For simplicity we may take the ground state $|0)$ to be unique but the usual two fold degeneracy has no effect on the result. There are N states $|i)$ with one "overturned spin" and energy $2q|J|$ above the ground state, which are connected to $|0)$ through the perturbation. Thus, the susceptibility at $T = 0$ is simply

$$\chi_\perp(0) = -\partial^2 E_0/\partial H_x^2 = Nm^2/q\,|J|. \tag{3.7}$$

States with two overturned spins have energy $4(q-1)|J|$ above E_0 if the spins are adjacent ($\frac{1}{2}qN$ states) or $4q|J|$ above E_0 if the spins are separated. Similarly with three spins[16] the lowest energy is obtained if all three spins are neighbors although this is only possible on a lattice with triangles ($p_3 \neq 0$). By considering these states, one readily finds

$$\chi_\perp(T) = \frac{Nm^2}{q\,|J|}\left\{1 + \frac{4}{q-2}e^{-2q|K|} + \frac{24p_3}{(q-2)(q-4)}e^{-4(q-1)|K|} + O(e^{-4q|K|})\right\}, \tag{3.8}$$

which shows that $\chi_\perp(T)$, in general, increases with T at low temperatures. (The mean-field approximation predicts that $\chi_\perp$ is constant up to $T = T_c$.)

The expansion (3.8) evidently breaks down when $q = 2$, that is, for the linear chain, and when $q = 4$ if $p_3 \neq 0$, as is the case for the kagomé lattice.

[16] We drop the adjective 'overturned' when it is obvious from the context.

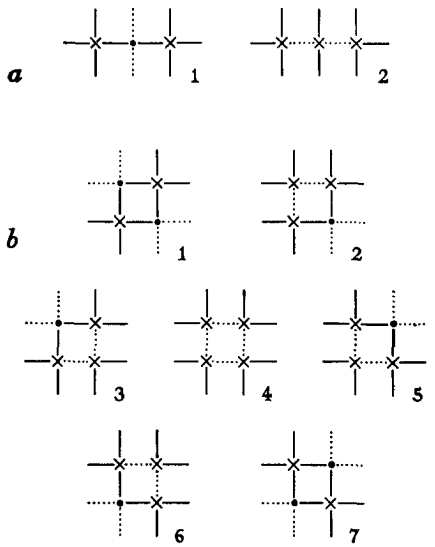

FIG. 2. Degenerate configuration of overturned spins (crosses) and 'wrong bonds' (solid lines) on the plane-square lattice.

This is because we have so far neglected the degeneracy of levels of different S^z. Thus, for the linear chain, any state with a row of adjacent overturned spins has the energy $E_0 + 4|J|$, while on the kagomé lattice a triangle of neighboring spins has the same energy as an adjacent pair. More generally, it is not difficult to see that degeneracy is certain to occur as soon as the states with $\frac{1}{2}q$ separated spins are considered (assuming q is even). For, if the $\frac{1}{2}q$ spins are all neighbors of a central site, the spin on the central site may be overturned without altering the energy. [Consider for example the configuration on the plane square lattice shown in Fig. 2(*a*).] When degeneracy occurs, the first-order formula (3.5) must be modified and the second term in (3.4) does not vanish. Consequently, terms of the form $e^{-A/T}/T$ appear in the expansion for $\chi_\perp$.

For a lattice of odd coordination number, like the honeycomb lattice ($q = 3$), such degeneracy cannot occur. The overturning of a single spin always alters the energy of a state and terms like $e^{-A/T}/T$ do not occur in the expansion.

To calculate the contribution to $\chi_\perp(T)$ from the degenerate states, one need only consider groups of degenerate states $|r)$ that are linked through the perturbation. The derivatives $\partial E_n/\partial H_x$ are then determined by the roots of the characteristic equation

$$|B_{rs} - \lambda\,\delta_{rs}| = 0, \tag{3.9}$$

where

$$B_{rs} = (r \mid \sum_i \sigma_i^z \mid s). \tag{3.10}$$

There is, however, no need to solve the equation explicitly since, from (3.3) and (3.4), we require only the sum of $\partial E_n/\partial H_z$ and of $(\partial E_n/\partial H_z)^2$ over the group of degenerate states. These sums are just proportional to the traces of the matrices $\mathbf{B}$ and $\mathbf{B}^2$, which are readily calculated.

To illustrate the method, consider the states of two overturned spins on the plane square lattice. These are coupled in two groups to states of three and four spins as shown diagramatically in Fig. 2. (Overturned spins are shown by crosses, and "wrong bonds," which determines the excitation energy, by solid lines.) Group (a) consists of two types of state which occur $2N$ times each, while group (b) comprises seven types occuring N times each. The matrices B_{rs} are readily seen to be

$$\mathbf{B}_a = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{3.11}$$

and

$$\mathbf{B}_b = \begin{bmatrix} \cdot & 1 & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & 1 & \cdot & 1 & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & 1 & 1 & \cdot \end{bmatrix} \tag{3.12}$$

where the dots indicate zeros. The traces of the matrices themselves vanish (which is an instance of a general result), but the traces of the squares are 2 and 16, respectively. The total contribution to the perpendicular susceptibility is thus

$$+20(Nm^2/kT)e^{-16|K|} \qquad \text{(plane square)} \tag{3.13}$$

and this will be the next term to dominate in the expansion (3.8).

For the three-dimensional tetrahedral (diamond) lattice, only states of type (a) arise and since there are $6N$ of these, the coefficient 20 in (3.13) becomes 12. For the ferromagnetic kagomé lattice the third term in (3.8) must, similarly, be replaced by

$$4(Nm^2/kT)e^{-12K} \qquad \text{(kagomé)}. \tag{3.14}$$

For the three-dimensional cubic lattices, further terms of (3.8) must be derived before the degenerate states need be considered.

For the closed linear chain (or ring) of N spins, where the second term in (3.8) is not valid, we must consider $N(N-1)$ states that may be labeled by the number $n = 1, 2, \cdots N-1$ of adjacent overturned spins and by the position $r = 1, 2, \cdots N$ of the first overturned spin. The matrix elements are clearly

$$B_{n,r;n',r'} = \delta_{n,n'+1}(\delta_{r,r'} + \delta_{r,r'-1}) + \delta_{n,n'-1}(\delta_{r,r'} + \delta_{r,r'+1}) \tag{3.15}$$

and so

$$\mathrm{Tr}\,\{\mathbf{B}^2\} = 4N(N-2). \tag{3.16}$$

We must now recall the two-fold degeneracy of the ground state[17] so that

$$\chi_\perp(T) = Nm^2/2\,|J| + 2N(N-2)m^2e^{-4|K|}/kT + \cdots. \tag{3.17}$$

The second term here is not proportional to N as would be expected on thermodynamic grounds. This implies that the analytic behavior at $T = 0$ in the limit $N \to \infty$ is not the same as for finite N. A similar situation arises with other properties of a linear ring of spins and may be regarded as indicative of a transition at $T_c = 0$. The true limiting behavior is revealed by the exact formula for $\chi_\perp(T)$ obtained in Sec. 5.

To close this section, we remark that the positive sign of the second term in (3.8), which leads to an increase of $\chi_\perp$ with rising temperature, is a direct consequence of the attraction between neighboring overturned spins. If this 'dynamic interaction' is ignored, as is done in simple spin wave theory, the coefficient $+4/(q-2)$ becomes -2 and the perpendicular susceptibility *falls* with increasing temperature. This is the situation for the 'superexchange' models,[18] in which magnetic spins on the bonds of a simple lattice interact indirectly through nonmagnetic spins on the sites (see also Sec. 5 below).

4. RELATION WITH CORRELATION FUNCTIONS

To relate the perpendicular susceptibility to the correlation functions, we first show that it is sufficient to calculate the partition function of a lattice with a *single* magnetic spin. This can be most directly seen from the graphical analysis of the complete partition function presented in Sec. 2. (For finite N the high-temperature expansion is convergent for all $T > 0$.) From the formula (2.5) it follows

[17] This analysis does not apply to an antiferromagnetic ring when N is odd, but the result for this case is given in Sec. 5.

[18] M. E. Fisher, Proc. Roy. Soc. (London) **A254**, 66 (1960); **A256**, 502 (1960).

that the second derivative $\partial^2 Z_N/\partial L_x^2$, which is needed to calculate the perpendicular susceptibility, has an expansion in terms of graphs involving only a single "doubled x spin." This doubled x spin may occur on any site, but in virtue of the translational symmetry of the lattice (wrapped on a torus), the contributions are independent of which site is occupied. Consequently,[19] in zero field

$$\frac{\partial^2 Z_N}{\partial L_x^2} = N\frac{\partial^2 Z_N^*}{\partial L_x^2} = 2N\frac{\partial Z_N^*}{\partial (L_x)^2}, \tag{4.1}$$

where $Z_N^*(K, L_x)$ is the partition function of a lattice of N spins in which the perpendicular field acts only on the spin at site 0. The perpendicular susceptibility is thus given by

$$\chi_\perp(T) = -\frac{\partial^2 F}{\partial H_x^2} = \frac{2Nm^2}{kT}\frac{\partial Z_N^*}{\partial (L_x)^2}\Big/ Z_N. \tag{4.2}$$

The partition function to be calculated is

$$Z_N^*(K, L_x) = \mathrm{Tr}^N\{\exp\,[K\sum_{(ij)}\sigma_i^z\sigma_j^z + L_x\sigma_0^x]\}. \tag{4.3}$$

(The analysis can actually be carried through in the presence of a *parallel* field H_z, but since the correlation functions in a parallel field are not readily evaluated, we omit this slight complication.) On introducing the spin variables $s_i = \pm 1$ for all sites but 0, this becomes

$$Z_N^* = \sum_{s_i=\pm 1}{}' \exp\,[K\sum_{(ij)}{}' s_i s_j] \times \mathrm{Tr}^1\left\{\exp\left[L_x\sigma_0^x + K\sum_{k=1}^{q}\sigma_0^z s_k\right]\right\}, \tag{4.4}$$

where the prime denotes that terms involving the site 0 are omitted and where s_k are the spin variables for the q sites neighboring 0. Now the trace in (4.4) is merely a special case of the generating function $\psi(\xi, \zeta)$ introduced in Eq. (2.7). Thus,

$$Z_N^* = \sum_{s_i=\pm 1}{}' \exp\,[K\sum_{(ij)}{}' s_i s_j]\psi\Big(L_x, K\sum_{k=1}^{q} s_k\Big). \tag{4.5}$$

On using the expression (2.10) for $\psi(\xi, \zeta)$, differentiating with respect to L_x^2 and putting $L_x = 0$, we obtain in zero field

$$\frac{\partial Z_N^*}{\partial (L_x)^2} = \sum_{s_i=\pm 1}{}' \exp\,[K\sum_{(ij)}{}' s_i s_j]\phi\Big(K\sum_{k=1}^{q} s_k\Big), \tag{4.6}$$

where

$$\phi(\zeta) = (\sinh\,\zeta)/\zeta. \tag{4.7}$$

[19] The argument can be put in more explicit form by introducing different fields on each site and then showing, along the lines of Sec. 2, that $\partial^2 Z_N/\partial L_{ix}\,\partial L_{jx}$ vanishes unless $i = j$. The total derivative $\partial^2 Z_N/\partial L_x^2$ is then given by (4.1), the second part following since Z_N involves only even powers of L_x.

We may now develop an argument familiar in connection with the generalized decoration and star-triangle transformations.[20] The function ϕ depends only on a finite number of spin variables s_k and can thus take only a finite number of distinct values. Consequently it may be expanded as a sum of products of the spin variables s_k. Rather than expand $\phi(K\sum s_k)$ itself, it proves more useful in most cases to write

$$\phi\Big(K\sum_{k=1}^{q} s_k\Big) = \tfrac{1}{2}\Upsilon_q(s_k)\sum_{s_0=\pm 1}\exp\left[K\sum_{k=1}^{q} s_0 s_k\right], \tag{4.8}$$

so that

$$\frac{\partial Z_N^*}{\partial (L_x)^2} = \tfrac{1}{2}\sum_{s_i=\pm 1}\exp\,[K\sum_{(ij)} s_i s_j]\Upsilon_q(s_k), \tag{4.9}$$

where the sums are now unrestricted and where

$$\Upsilon_q(s_1, s_2, \cdots s_q) = \tanh\left[K\sum_{k=1}^{q} s_k\right]\Big/ K\sum_{k=1}^{q} s_k. \tag{4.10}$$

Since $\Upsilon_q(s_1, \cdots s_q)$ is invariant under the operation $s_k \to -s_k$ (all k), we may omit products with an odd number of factors and expand in the form

$$\Upsilon_q(s_1, \cdots s_q) = C_0^q + C_1^q\sum_{(kl)} s_k s_l + C_2^q\sum_{(klmn)} s_k s_l s_m s_n + \cdots, \tag{4.11}$$

where the sums run over the $\binom{q}{2r}$ distinct products of r factors formed from the q variables s_k. As the s_k run through the 2^q possible different combinations the identity (4.11) yields 2^q equations which can be used to determine the coefficients C_r^q of which there are $[\frac{1}{2}q] + 1$ in all[21]: In the present case, many of these equations are redundant, but all are required in the more general case in which different bonds have different strengths so that $K\sum s_k$ in (4.10) is replaced by $\sum K_k s_k$.

To evaluate C_r^q explicitly, we multiply (4.11) by the product $s_1 s_2 \cdots s_{2r}$ and sum over all values of the s_k. Any term on the right-hand side that contains an unpaired factor s_k will vanish when the sum over $s_k = \pm 1$ is performed, so that finally only the single term matching the product $s_1 s_2 \cdots s_{2r}$ survives. On rewriting and using (4.10), the general result for the coefficients is found to be

$$C_r^q(K) = 2^{-q}\sum_{s_k=\pm 1}\Big(\prod_{l=1}^{2r} s_l\Big)\tanh\left[K\sum_{k=1}^{q} s_k\right]\Big/ K\sum_{k=1}^{q} s_k. \tag{4.12}$$

[20] M. E. Fisher, Phys. Rev. **113**, 969 (1959).

[21] The notation $[x]$ denotes the greatest integer contained in x.

where $r = 0, 1, 2, \cdots \frac{1}{2}q$ and where the empty product is assigned the value unity. An obvious generalization of this method yields the coefficients when the bonds have different interaction energies.

For the sake of reference, we tabulate below the detailed expressions for $C_r^q(K)$ in the cases $q = 2$, 3, and 4. With the notation

$$\tau(K) = (1/K) \tanh K \tag{4.13}$$

these are

$$\begin{aligned} C_0^2 &= \tfrac{1}{2}[\tau(2K) + 1], \\ C_1^2 &= \tfrac{1}{2}[\tau(2K) - 1], \end{aligned} \tag{4.14}$$

$$\begin{aligned} C_0^3 &= \tfrac{1}{4}[\tau(3K) + 3\tau(K)], \\ C_1^3 &= \tfrac{1}{4}[\tau(3K) - \tau(K)] \end{aligned} \tag{4.15}$$

and

$$\begin{aligned} C_0^4 &= \tfrac{1}{8}[\tau(4K) + 4\tau(2K) + 3], \\ C_1^4 &= \tfrac{1}{8}[\tau(4K) - 1], \\ C_2^4 &= \tfrac{1}{8}[\tau(4K) - 4\tau(2K) + 3]. \end{aligned} \tag{4.16}$$

To complete the calculation of $\chi_\perp(T)$, the expansion (4.11) is substituted in (4.9) and thence into (4.2). This yields the final result

$$\chi_\perp(T) = \frac{Nm^2}{kT}\{C_0^q(K) + C_1^q(K) \sum_{(kl)} \langle s_k s_l \rangle + C_2^q(K) \sum_{(klmn)} \langle s_k s_l s_m s_n \rangle + \cdots\}, \tag{4.17}$$

where the zero-field spin correlation functions $\langle s_k s_l \rangle$, $\langle s_k s_l s_m s_n \rangle$, $\cdots$ between the q spins neighboring the site 0, are defined in the standard way through the formula (3.3). (As before, the sums run over all possible combinations of the q spins). This formula expresses $\chi_\perp$ in terms of short-range spin correlations of order up to q (or $q - 1$ if q is odd). We show below, however, that the correlation function of maximal order when q is even can be expressed in terms of those of order $q - 2$ and less. The coefficients $C_r^q(K)$ and all their derivatives are smoothly varying, so that any anomalies in $\chi_\perp(T)$ are consequences of similar anomalies in the correlation functions.

By expanding the correlation functions at high and low temperatures, one may derive alternative expansions for $\chi_\perp$ to those found in the previous sections. If one expands $\phi(K\sum s_k)$, rather than $\Upsilon_q(s_k)$, in spin products one obtains a slightly different expression for $\chi_\perp$ in terms of the zero-field properties of a lattice with the spin on site 0 completely uncoupled from the neighboring spins. Denoting the properties of this lattice by a dagger the result is

$$\chi_\perp(T) = \frac{Nm^2}{kT}\frac{Z_N^\dagger}{Z_N}\{D_0^q + D_1^q \sum_{(kl)} \langle s_k s_l \rangle^\dagger + D_2^q \sum_{(klmn)} \langle s_k s_l s_m s_n \rangle^\dagger + \cdots\}, \tag{4.18}$$

where the coefficients $D_r^q(K)$ are given by the expressions (4.12) to (4.15) with tanh replaced by sinh and $\tau(K)$ by $\phi(K)$. This formula is a little simpler to expand at high temperatures and can be used to get a compact expression for the perpendicular susceptibility of the Bethe lattices (see next section).

5. DETAILED RESULTS

We first verify the behavior at high and low temperatures found in Secs. 2 and 3. At high temperatures the standard methods of expansion[8,13] show that the correlations fall off as J/kT or faster. On the other hand, by (4.12) the zeroth coefficient is

$$C_0^q(K) = 2^{-q} \sum_{s_k = \pm 1} \tau\Big(K \sum_{k=1}^{q} s_k\Big), \tag{5.1}$$

$$= 2^{-q} \sum_{t=0}^{q} \binom{q}{t} \tau[K(q - 2t)]. \tag{5.2}$$

At high temperatures $K \to 0$ and $\tau(K) = 1 - \frac{1}{3}K^2 + O(K^4)$ so that

$$C_0^q(K) = 1 - O(K^2), \tag{5.3}$$

and it follows immediately from (4.12) that all the higher coefficients vanish at least as fast as K^2. From (4.17) we thus obtain generally

$$\chi_\perp(T) = \frac{Nm^2}{kT}\{1 - O(K^2)\} \qquad (T \to \infty) \tag{5.4}$$

in agreement with (2.13).

At low temperatures all the correlation functions approach $+1$ as $\exp(-A/T)$ provided the lattice orders ferro- or antiferromagnetically. Thus,

$$\chi_\perp(T) \approx \frac{Nm^2}{kT} \sum_{r=0}^{[(q+1)/2]} C_r^q(K) \binom{q}{2r} \tag{5.5}$$

$$\approx \frac{Nm^2}{kT}\frac{\tanh qK}{qK} = \frac{Nm^2}{qJ} \tanh qK \quad (T \to 0), \tag{5.6}$$

where the second line follows by putting all $s_k = 1$ in the formulas (4.10) and (4.11). Taking the limit $K \to \pm\infty$ confirms the result (3.7). It also immediately follows from the form of the coefficients $C_r^q(K)$ that there are no terms of the type $e^{-A/T}/T$ in the low-temperature expansion of $\chi_\perp(T)$ if q is odd, in agreement with the previous conclusion. [Compare formulas (4.14), (4.15), and (4.16)].

Linear Chain

For a one-dimensional ring or chain of spins $q = 2$, so that by (4.13) and (4.17)

$$\chi_\perp(T) = (Nm^2/2kT) \times \{1 + \tau(2K) + [\tau(2K) - 1]\langle s_1 s_2\rangle\}, \quad (5.7)$$

where $\langle s_1 s_2\rangle$ is the second-neighbor spin correlation function. By using the Oguchi-van der Waerden method of expansion this is seen to be

$$\langle s_1 s_2\rangle = (v^2 + v^{N-2})/(1 + v^N), \quad (5.8)$$

where

$$v = \tanh K \quad (5.9)$$

and where we have assumed the chain of N spins is closed. (Otherwise the terms in v^{N-2} and v^N are absent). Taking the limit $N \to \infty$ for fixed $T > 0$, yields for the limiting perpendicular susceptibility per spin,[22]

$$\chi_\perp(T)/N = (m^2/2|J|)(\tanh |K| + |K| \operatorname{sech}^2 K), \quad (5.10)$$

which may be compared with the corresponding expression for the parallel susceptibility, namely,

$$\chi_\parallel(T)/N = \frac{m^2}{kT}\frac{1+v}{1-v} = \frac{m^2}{|J|} K e^{2K}. \quad (5.11)$$

The result (5.10) is plotted in Fig. 3 (curve a) in terms of the reduced dimensionless variables

$$\theta = 1/qK = kT/q|J| \quad (5.12)$$

and

$$X = \chi(q|J|/Nm^2). \quad (5.13)$$

(Note the restricted extent of the vertical and horizontal scales in Fig. 3). Whereas the antiferromagnetic parallel susceptibility has a low broad maximum at $\theta = 1.000$ of magnitude $X_\parallel = 0.3679$, the perpendicular susceptibility attains a relatively high and narrow maximum,

$$\chi_{\perp\max}/\chi_\perp(0) = 1.1997, \quad (5.14)$$

at the much lower temperature $\theta = 0.41677$, before dropping to the value $X_\perp = 1$ at $T = 0$.

At low temperatures the perpendicular susceptibility of the infinite chain has the expansion

$$\lim_{N\to\infty}\frac{\chi_\perp}{N} = \frac{m^2}{2|J|}\{1 - 2e^{-2|K|} + 2e^{-4|K|} - \cdots\} + (2m/kT)e^{-2|K|}\{1 - e^{-4|K|} + \cdots\}. \quad (5.15)$$

[22] Since the development of the general theory[12] this formula has been rederived by S. Katsura, Phys. Rev. **127**, 150, 8 (1962), who has obtained, among other interesting results, an exact solution for a linear chain in an arbitrary perpendicular field.

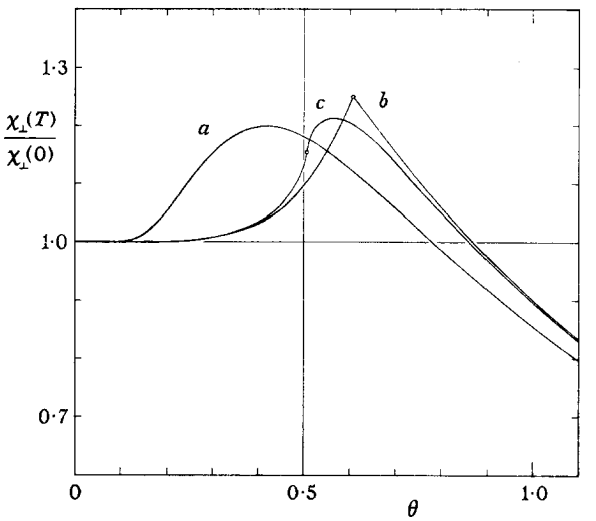

FIG. 3. Perpendicular susceptibilities of (a) the linear chain, (b) the $q = 3$ Bethe lattice, and (c) the plane honeycomb lattice in the vicinity of the maximum. (Note the restricted range of the vertical scale.)

Comparison with Eq. (3.17) shows, as anticipated, that the leading term of the temperature dependence is not of the same form as for a finite chain. We may verify and extend the previous result for finite N by expanding (5.7) and (5.8) directly, which yields

$$\chi_\perp(T) = \frac{Nm^2}{2|J|}\{1 - 2^*(N-1)e^{-4|K|} + O(N^2e^{-8|K|})\} + (Nm^2/kT)2^*(N-2)e^{-4|K|}\{1 + O(Ne^{-4K})\} \quad (5.16)$$

for the cases $J > 0$ (all N) or $J < 0$ and N is even. The asterisks indicate that when $J < 0$ and N is odd the coefficient 2 becomes $\frac{2}{3}$.

Bethe Lattices

Before discussing two-dimensional lattices we consider a class of pseudolattices for which Bethe's statistical approximation is exact. These are the Bethe lattices,[13] that is, infinite homogeneous Cayley trees which are completely characterized by the coordination number q. (For $q = 2$ we regain the linear chain.) The critical point is determined by the equation

$$|v_c| = \tanh |K_c| = 1/(q-1) \quad (5.17)$$

and the parallel susceptibility is given by the Firgau formula[13]

$$\chi_\parallel(T) = \frac{Nm^2}{kT}\frac{1 + \tanh K}{1 - (q-1)\tanh K} = \frac{Nm^2}{J}\frac{2K}{qe^{-2K} - q + 2}. \quad (5.18)$$

To derive the perpendicular susceptibility above the critical temperature, we use the expression (4.18) which refers to a "dagger" lattice with a single uncoupled spin. Above T_c the van de Waerden expansion now shows that

$$Z_N^{\dagger}/Z_N = (\cosh K)^{-q}, \qquad (K < K_c) \tag{5.19}$$

since there are q missing bonds in the dagger lattice. Similarly, since there are no closed circuits in the Bethe lattice, the spins neighboring the uncoupled spin 0 are completely uncorrelated, so that

$$\langle s_k s_l \rangle = \langle s_k s_l s_m s_n \rangle = \cdots = 0. \tag{5.20}$$

Thus, from (4.18) and (5.2) we obtain the explicit expression

$$\chi_\perp(T) = \frac{Nm^2}{J} (2 \cosh K)^{-q} \sum_{t=0}^{q} \binom{q}{t} \frac{\sinh K(q-2t)}{(q-2t)}, \qquad (T > T_c) \tag{5.21}$$

$$= \frac{Nm^2}{J} \int_0^K (\cosh K'/\cosh K)^q \, dK'. \tag{5.22}$$

From this it follows (for $q > 2$) that $\chi_\perp(T)$ falls *monotonically* as T rises above T_c.

At the critical point we find

$$q = 3, \quad \chi_\perp(T_c)/\chi_\perp(0) = \tfrac{5}{4} = 1.250, \tag{5.23}$$

and

$$q = 4, \qquad = \tfrac{7}{9} + \tfrac{16}{27} \ln 2 = 1.18853, \tag{5.24}$$

while for large q it is easy to show that

$$\lim_{q \to \infty} \frac{\chi_\perp(T_c)}{\chi_\perp(0)} = 1. \tag{5.25}$$

This is just the result of the mean-field approximation. More generally, in the limit $q = \infty$ we find, in terms of the reduced variables defined above,

$$X_\perp = 1/\theta, \qquad \theta > \theta_c = 1, \tag{5.26}$$

which is the value for a completely free spin, while for the parallel susceptibility

$$X_\parallel = 1/(\theta \mp 1) \tag{5.27}$$

as $J > 0$ or $J < 0$, respectively.

Below T_c we cannot use these formulas since the lattice orders and the high-temperature expansions in v are not valid. In fact the correlation functions have a discontinuity in gradient at T_c similar to that in the energy.[13] It follows that the gradient of $\chi_\perp(T)$ changes sign discontinuously at T_c and $\chi_\perp(T)$ falls monotonically again as T drops below T_c. One cannot now derive explicit general expressions for $\chi_\perp(T)$ since the correlation functions are dependent on the solution of an algebraic equation.[13] For the $q = 3$ Bethe lattice, however, we obtain, with the aid of a transformation of the correlation function $\langle s_1 s_2 \rangle$ (see below and reference 20),

$$\chi_\perp(T) = (Nm^2/3\,|J|) \tanh^2 K \times \{3 \coth |K| + \tanh |K| - 3\omega_1(K)\} \tag{5.28}$$

where

$$\omega_1(K) = 1 - 4/(e^{4|K|} - 1)(e^{2|K|} - 2) \quad (T \leq T_c) \tag{5.29}$$

$$= \tanh |K|. \qquad (T \geq T_c). \tag{5.30}$$

The behavior of $\chi_\perp(T)$ in the critical region for this case is shown in Fig. 3 (curve *b*).

Honeycomb Lattice

For the plane honeycomb lattice the coordination number is $q = 3$ and to use the result (4.12) we need only the second-neighbor pair correlation functions $\langle s_1 s_2 \rangle$, $\langle s_2 s_3 \rangle$, and $\langle s_1 s_3 \rangle$, which by symmetry, are equal to one another. The second-neighbor correlation has not been calculated explicitly for the honeycomb lattice but by the theory of transformations[20] it is readily expressed in terms of the first-neighbor correlation $\langle s_0 s_1 \rangle$ which is simply proportional to the energy of the lattice. Thus, by Eqs. (81) and (82) of reference 20 we have

$$\langle s_1 s_0 \rangle = \alpha(\langle s_1^2 \rangle + \langle s_1 s_2 \rangle + \langle s_1 s_3 \rangle) + \beta \langle s_1^2 s_2 s_3 \rangle, \tag{5.31}$$

where

$$\alpha = \tfrac{1}{4}[\tanh 3K + \tanh K],$$
$$\beta = \tfrac{1}{4}[\tanh 3K - 3 \tanh K]. \tag{5.32}$$

Now $s_1^2 = 1$, so that solving for the second-neighbor correlation yields

$$\langle s_1 s_2 \rangle = \tfrac{1}{2}(\coth K + 3 \tanh K)\langle s_0 s_1 \rangle - \tfrac{1}{2}(1 + \tanh^2 K). \tag{5.33}$$

The perpendicular susceptibility is then given by Eq. (5.28) above, but with

$$\omega_1(K) = \langle s_0 s_1 \rangle = -U_H(K)/\tfrac{1}{2}qJ \tag{5.34}$$

where $U_H(K)$ is the energy per site of the honeycomb lattice which has been calculated explicitly by Houtappel.[6]

The behavior of the perpendicular susceptibility of the honeycomb lattice in the critical region is compared with that of the corresponding Bethe lattice in Fig. 3. The critical point for the honeycomb (marked by a circle) is given by

$$\chi_\perp(T_c)/\chi_\perp(0) = 2/\sqrt{3} = 1.15470,$$
$$\theta_c = kT_c/3|J| = 0.50622. \quad (5.35)$$

At T_c the gradient of the susceptibility exhibits a logarithmic singularity, the behavior in the neighborhood being

$$\chi_\perp(T) \approx (Nm^2/3|J|)\{1.1547 + 0.4840[1 - (T/T_c)] \ln |1 - (T/T_c)|\}. \quad (5.36)$$

In contrast to the Bethe lattice, the perpendicular susceptibility of the honeycomb lattice exhibits a rounded maximum 10% above T_c, of magnitude $\chi_{\perp\max} = 1.213\chi_\perp(0)$. At high and low temperatures the values for the two lattices approach asymptotically, as might be expected.

Square Lattice

For the plane square lattice the coordination number is $q = 4$ and to use the result (4.12) we need the three distinct correlation functions

$\omega_2(K) = \langle s_1 s_2\rangle$, second-neighbor pair,
$\omega_3(K) = \langle s_1 s_3\rangle$, third-neighbor pair,
$\Omega(K) = \langle s_1 s_2 s_3 s_4\rangle$, fourth order, all first neighbors of a site.

The first of these, the second-neighbor pair correlation, has been calculated explicitly by Onsager and Kaufman.[4] Applying a Landen transformation to their result, we obtain a formula valid for all T, namely,

$$\omega_2(K) = (1/\pi)\coth^2 2K\,[E(k_1) + k_1'' K(k_1)], \quad (5.37)$$

where

$$k_1 = 2\tanh 2K/\cosh 2K,$$
$$k_1'' = 2\tanh^2 2K - 1, \quad (5.38)$$

and where $E(k)$ and $K(k)$ are the complete elliptic integrals of modulus k as defined, for example, by Jahnke and Emde.[23] Onsager and Kaufman obtained an expression for the third-neighbor pair-correlation function in terms of two determinents involving integrals, which they show can generally be transformed into complete elliptic integrals but they do not give any explicit formulas. Potts and Ward,[24] on the other hand, express $\langle s_1 s_3\rangle$ in terms of a single determinent which is easier to evaluate although the analysis is still rather involved. We find

$$\omega_3(K) = \tfrac{1}{2}\coth^2 2K - (2/\pi k_1)^2 \times [E^2(k_1) - 2k_1'' K(k_1)E(k_1) + (k_1'')^3 K^2(k_1)]. \quad (5.39)$$

[23] E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, New York, 1945).
[24] R. B. Potts and J. C. Ward, Progr. Theoret. Phys. (Kyoto) **13**, 38 (1955).

No fourth-order correlation functions have been evaluated for the Ising model, although it should be possible to do so along the lines used by Onsager and Kaufman[4] or, more readily, by extending the combinatorial method of Potts and Ward.[24] In the present instance, however, we can avoid this as for the honeycomb lattice above by using the transformation theory.[20] The first-neighbor correlation function

$$\omega_1(K) = \tfrac{1}{2}\coth 2K\,[1 + (2/\pi)k_1'' K(k_1)], \quad (5.40)$$

which is just proportional to the energy,[2,4] is expanded in terms of correlations in the first-neighbor shell. Solving for the fourth-order function yields, after some reduction, the explicit relation

$$\Omega(K) = \langle s_1 s_2 s_3 s_4\rangle = 1 + 2\coth^2 2K - 4\coth 2K\,(1 + \coth^2 2K)\langle s_0 s_1\rangle + 2\coth^2 2K\,[2\langle s_1 s_2\rangle + \langle s_1 s_3\rangle]. \quad (5.41)$$

In passing, we mention that a similar formula holds for the kagomé lattice (which has the same coordination number) if the term $2\langle s_1 s_2\rangle$ is replaced by $\langle s_0 s_1\rangle + \langle s_1 s_4\rangle$. In this case, however, the two second-neighbor pair-correlation functions $\langle s_1 s_3\rangle$ and $\langle s_1 s_4\rangle$ are not yet known explicitly. With the decoration and star-triangle transformations[20] they can be expressed in terms of the two third-neighbor correlation functions on the honeycomb lattice, but these are also not known explicitly at present.

Combining the formulas (4.16) and (4.17) yields

$$\chi_\perp(T) = (Nm^2/4J)\{\tfrac{1}{8}\tanh 4K + \tanh 2K + \tfrac{3}{2}K + (\tfrac{1}{4}\tanh 4K - K)[2\omega_2(K) + \omega_3(K)] + (\tfrac{1}{8}\tanh 4K - \tanh 2K + \tfrac{3}{2}K)\Omega(K)\}, \quad (5.42)$$

so that on substituting the results (5.37) to (5.41), we finally have an explicit expression for the perpendicular susceptibility of the plane-square lattice.

On using the critical values

$$\theta_c = 0.567296,$$
$$\omega_1(K_c) = \tfrac{1}{2}\sqrt{2} = 0.707107,$$
$$\omega_2(K_c) = 2/\pi = 0.636620, \quad (5.43)$$
$$\omega_3(K_c) = 1 - (4/\pi^2) = 0.594715,$$
$$\Omega(K_c) = (4/\pi)^2(\pi - 1) - 3 = 0.471819,$$

we find

$$\chi_\perp(T_c)/\chi_\perp(0) = 1.13695, \quad (5.44)$$

which is slightly smaller than for the honeycomb

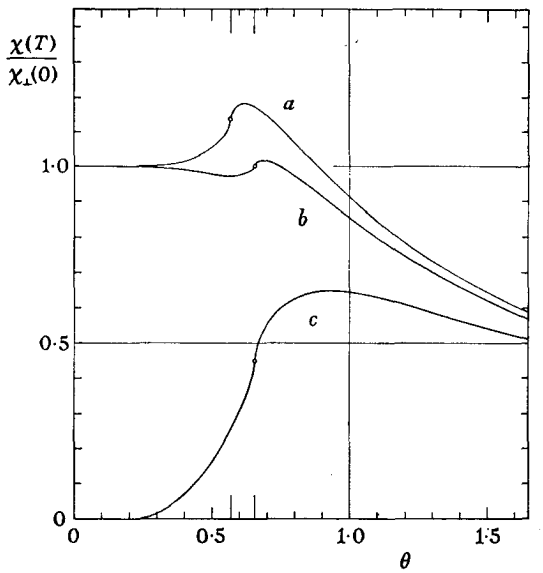

FIG. 4. Perpendicular susceptibilities of (a) the plane square lattice and (b) the plane super-exchange lattice. Curve (c) is the parallel susceptibility of the superexchange, model.

lattice. The gradient $\partial\chi_\perp/\partial T$ again exhibits a symmetric logarithmic singularity since, near T_c,

$$[\chi_\perp(T) - \chi_\perp(T_c)]/\chi_\perp(0) \approx 0.470172\,[1 - (T/T_c)]\ln|1 - (T/T_c)|. \quad (5.45)$$

The parameters of the maximum which occurs above T_c are

$$T_{\max}/T_c = 1.0887, \quad \chi_{\perp\max}/\chi_\perp(0) = 1.18314, \quad (5.46)$$

so that the maximum is slightly lower and closer to the critical point than it is for the honeycomb lattice. The values in (5.44) and (5.46) may be compared with the corresponding (estimated) values for the *parallel* antiferromagnetic susceptibility which are[8,9]

$$(4|J|/Nm^2)\chi_\parallel(T_c) = 0.2768,$$
$$T_{\max}/T_c = 1.5371, \quad (4|J|/Nm^2)\chi_{\parallel\max} = 0.42957. \quad (5.47)$$

A graph of $\chi_\perp(T)$ for the square lattice is given in Fig. 4 where it is compared with the results for the plane superexchange lattice[18] (see below).

Plane Triangular Lattice

In this case, both sixth-order and fourth-order correlation functions are required. The sixth-order function $\langle s_1 s_2 s_3 s_4 s_5 s_6\rangle$ can, as above, be expressed in terms of second- and fourth-order functions, but expressions for these are not known at present.

Three-dimensional Lattices

To obtain accurate quantitive estimates of $\chi_\perp(T)$ for the three-dimensional lattices in the critical region, it is necessary to either extend the low- and high-temperature series expansions appreciably, or to obtain moderately long expansions of the required multiple correlation functions. We may draw some general conclusions however, on the basis of the study of other properties of the three-dimensional lattices that reveal the trend of critical behavior as the dimensionality is increased.[7,8,13] In particular, we expect the critical anomalies in three dimensions to be less pronounced and to be asymmetric above and below T_c. At low temperatures, $\chi_\perp(T)$ will rise more slowly and $\chi_\perp(T_c)/\chi_\perp(0)$ will be closer to unity than in two dimensions. At the critical point, $\partial\chi_\perp/\partial T$ should again become infinite but less strongly, especially above T_c. The maximum in $\chi_\perp(T)$ should be relatively much lower and will probably occur only some 1% or 2% above the critical point.

Superexchange Lattices

To complete our investigation of the perpendicular susceptibility of the Ising model, we discuss the antiferromagnetic superexchange lattices,[18] which in two dimensions are exactly soluble even in a magnetic field. One of the simplest examples is a decorated square lattice in which magnetic spins (of coordination number $q = 2$) on the bonds of the lattice are coupled antiferromagnetically through *non*-magnetic spins on the vertices of the lattice.[18] By the use of the generalized decoration transformation,[20] the partition function of this lattice in a field can be related to that of the normal square lattice in zero field. The properties of this superexchange lattice in a *parallel* field have been discussed in detail[18] but by using the results (2.7) and (2.10) the theory is easily extended to include a perpendicular field as well. The partition function for a superexchange lattice of N magnetic spins is found to be

$$Z_N(K, L_x, L_z) = [f(K, L_x, L_z)]^N Q_{N/2}\{G(K, L_x L_z)\}, \quad (5.48)$$

where $Q_M(K)$ is the partition function for a standard plane square lattice of M vertices in zero field and where

$$e^{4G} = \frac{\cosh\left[(2K + L_z)^2 + L_x^2\right]^{1/2} \cosh\left[(2K - L_z)^2 + L_x^2\right]^{1/2}}{\cosh^2 (L_x^2 + L_z^2)^{1/2}}, \tag{5.49}$$

and

$$f = 2e^G \cosh (L_x^2 + L_z^2)^{1/2}. \tag{5.50}$$

From the partition function we find, in the standard way, that the zero-field perpendicular susceptibility is

$$\chi_\perp(T) = \tfrac{1}{2}(Nm^2/2J)\{\tanh 2K[1 + \omega_1(G)] + K[1 - \omega_1(G)]\}, \tag{5.51}$$

where $\omega_1(K)$ is given by (5.40). The magnetic anisotropy can be written

$$\chi_\perp - \chi_\parallel = \tfrac{1}{4}(Nm^2/2J)\mathfrak{u}(K)[1 - 4K/\sinh 4K], \tag{5.52}$$

where

$$\mathfrak{u}(K) = 2 \tanh 2K\,[1 + \omega_1(G)] \tag{5.53}$$

is the (reduced) energy of the super-exchange lattice.

At low temperatures we have the expansion

$$\chi_\perp(T) = (Nm^2/2|J|)\{1 - 2e^{-4|K|} + O(e^{-8|K|}/kT)\} \tag{5.54}$$

so that, in contrast to most other lattices, the perpendicular susceptibility *falls* as the temperature rises from zero (see Sec. 3). As can be seen from Fig. 4, the susceptibility then passes through a shallow minimum at 14% below T_c [$\chi_{\perp\min}/\chi_\perp(0) = 0.972$] before rising steeply to attain a vertical tangent at the critical point

$$\theta_c = 0.654206, \tag{5.55}$$

where we have

$$\chi_\perp(T_c)/\chi_\perp(0) = 1.00074. \tag{5.56}$$

The perpendicular susceptibility then rises to a relatively low and sharp maximum at 4.3% above T_c where $\chi_{\perp\max}/\chi_\perp(0) = 1.018$. The *parallel* susceptibility is also shown in Fig. 4 for the purpose of comparison.

Finally we mention that the partition function of the semimagnetic honeycomb lattice[25] in an arbitrary perpendicular field can be derived in closed form from the zero-field partition function of the triangular lattice by employing the generalized star-triangle transformation[20] with transformation function

$$\psi(s_1, s_2, s_3) = 2 \cosh\left[K^2(s_1 + s_2 + s_3)^2 + L_x^2\right]^{1/2}. \tag{5.57}$$

ACKNOWLEDGMENTS

The author is indebted to Dr. I. J. Zucker for performing the numerical evaluation of the perpendicular susceptibility of the square lattice on the computer at the Northampton College of Advanced Technology. The interest and advice of Professor C. Domb and Dr. M. F. Sykes is gratefully acknowledged.

[25] In the semimagnetic honeycomb lattice the spins on alternate sites have zero magnetic moment. This lattice was first considered by S. Naya, Progr. Theoret. Phys. (Kyoto) **11**, 53 (1954), in relating the magnetization of the triangular and honeycomb lattices.

Quaternionic Representations of Compact Groups

D. FINKELSTEIN*
Yeshiva University, New York
J. M. JAUCH
University of Geneva and CERN, Geneva, Switzerland
AND
D. SPEISER†
University of Geneva, Geneva, Switzerland
(Received 20 July 1962)

The main purpose of this paper is to show the conditions under which a finite dimensional representation of a group, irreducible over the complex field, is reducible over quaternions. The answer is simply stated in terms of the Frobenius-Shur classification of group representations.

I. INTRODUCTION

IN this note the attempt is made to formulate a theory of representations of groups over the skew-field of the quaternions. The whole approach is based on spectral resolution techniques which apply in the same way to the fields of real numbers, complex numbers and quaternions. It is therefore a *direct way* without the detour of transcribing the quaternion operators into complex ones through the use of the Pauli matrices. This way was described in a previous paper,[1] to which this note is a sequel.

Elsewhere[2] the particular case SU_2 (2×2, unitary, determinant = 1) has been investigated in detail. In Sec. II, we recall some notions and theorems of the spectral theory of operators in a Q Hilbert space. In Sec. III the basic concepts of a representation over the quaternions are developed and the main tools and lemmas are generalized, so that they do not depend upon the commutativity of the underlying field. Finally, in Sec. III.6, the main reduction theorem is formulated and proved. This theorem answers the question: When does a representation, irreducible over the field of complex numbers, reduce over the quaternions? This question is central, for the complex numbers are embedded in the quaternions as a subfield, and the problem of finding all complex representations (of finite degree) is, in principle, completely solved. It will be shown that this question has a straightforward answer in terms of the well-known tripartite classification of irreducible representations given by Frobenius and Schur[3] (see also Wigner[4]). The preparatory Sec. III.4 is devoted to an exposition of their results.

A well-known theorem (cf. Pontrjagin,[5] p. 282) says that every connected, compact group is the factor group of a direct product of simple groups over a discrete normal subgroup.

It is therefore enough to know which representations of the simple groups reduce over Q. Since the classification explained in Sec. III.4 has been applied to all simple groups, we do not enter into this subject. It will also be treated in a forthcoming paper by one of the authors from a different point of view.

This paper deals only with compact groups and therefore with finite dimensional unitary representations. We hope to return to the non-compact groups elsewhere. On the other hand the extension of the results presented here to infinite dimensional unitary representations is straightforward.

Notation

C, Q: the fields of complex numbers and quaternions.

M^H: Hermitian conjugate
M^T: transposed
M^Q: quaternion conjugate (if the m_{ik} are quaternions)
M^*: complex conmugate (if the m_{ik} are complex numbers)
M^A: adjoint = M^{-1T} of M.

* Supported by the National Science Foundation.
† Supported by the Swiss National Foundation.

[1] Foundations of Quaternion Quantum Mechanics, D. Finkelstein, J. M. Jauch, S. Schiminovitch, D. Speiser. J. Math. Phys. 3, 1962, p. 207.

[2] Notes on Quanternion Quantum Mechanics II, III, D. Finkelstein, J. M. Jauch, D. Speiser. CERN 59-9, 59-17, 1959.

[3] G. Frobenius und J. Schur: über die reellen Darstellungen der endlichen Gruppen. Sitzungsbericht des Königl. Pr. Akademie der Wissenschaften, 1906, B II, p. 186.

[4] E. P. Wigner: Group theory and its applications to the Quantum Mechanics of Atomic Spectra, New York and London, 1959, p. 285.

[5] L. Pontrjagin: *Topological Groups*, 1946.

Subscripts (e.g., q_1) denote the components of a quaternion:

$$q = q_0 + q_1 i_1 + q_2 i_2 + q_3 i_3 .$$

Where a matrix is decomposed in two complex matrices, we write

$$M = M_0 + M_2, [M_0, i_3]_- = [M_2, i_3]_+ = 0,$$

No confusion will arise between these subscripts 0, 2 and the ones mentioned before $0 \cdots 3$

II. SOME NOTIONS AND THEOREMS OF THE SPECTRAL THEORY OF OPERATORS IN A Q SPACE

For a detailed development of a theory of operators in a Q space, and for the proofs of the following statements we refer to references 1 and 2. Here, we merely state the existence of a spectrum for Hermitian and unitary operators.

1. Every Hermitian (quaternionic) matrix H can be completely diagonalized and all eigenvalues of H are real numbers.

2. Every unitary (quaternionic) matrix U, $U^{-1} = U^H$, can be completely diagonalized with all diagonal elements of the form $e^{i_3\varphi}$ where $0 \leq \varphi \leq \pi$. The set of the resulting diagonal elements is uniquely determined by U. (Note that only half of the φ circle is used.)

3. To every n-dimensional Q space can be associated a $2n$-dimensional C space. To every Q operator then is associated a C operator. This association is biunique and called the symplectic representation. Details are presented elsewhere.[1,2,6]

III. Q REPRESENTATIONS

In the same way as in the theory of C representations we give the following definition: A *Q representation* of a (topological) group G is a homomorphic mapping of G into a (topological) group of linear operators on a Q space (cf. reference 5, p. 110). In the same way as in the complex theory (by Hurwitz integration over Hermitian form), one proves that every representation of a compact group is equivalent to a representation by unitary matrices. In the following we shall speak therefore always of unitary representations $D(G)$ for which $D^A \equiv D^{-1T} = D^{HT} = D^*$.

We note that by identifying i with i_3 every C representation is already a Q representation. *However, even if a C representation is irreducible, the associated Q representation need not be so.* It is the main purpose of this paper to indicate when and how a representation, irreducible over C, reduces over Q. This section contains the definitions of some generalized concepts and the generalizations of the well known lemmas.

1. Character and Trace

In the complex case, one defines the character by means of the trace (= diagonal sum) of a matrix. This definition is motivated by the equality

$$\text{Tr } (A) = \text{Tr } (B^{-1}AB), \qquad A, B \text{ complex matrices}$$

which expresses the fact that the character of a representation is independent of its matric expression; and also that the character is a class function, i.e., all group elements which can be transformed into each other have the same character. In a quaternion space this is no longer true for the diagonal sum Tr. For example, take a one-dimensional (even unitary) matrix $= i_3$, and $B = i_1$. Then $(-i_1)i_3(i_1) = -i_3$, so

$$\text{Tr } A \neq \text{Tr } B^{-1}A\,B.$$

But we observe that $\text{Re (Tr } A) = \text{Re (Tr } B^{-1}AB)$. Therefore we shall define the character

$$X(M) = \text{Re (Tr } M):$$

(a) $X(M)$ belongs to the center of the field for all M,
(b) $X(A + B) = X(A) + X(B)$,
(c) $X(AB) = X(BA)$.

Sometimes it is convenient to have a definition which is uniform for representations over all three fields R, C, Q by defining

$$X(M) \equiv \text{av}_U\, U^{-1}MU,$$

where av_U involves integration over the quaternionic unitary (= symplectic) group (which of course is a compact group): i.e.,

$$X(M) = \frac{\int U^{-1}MU\, d_\mu(U)}{\int d_\mu(U)}.$$

For the characters $X_1(g)$, $X_2(g)$ of two representations $D_1(g)$, $D_2(g)$, defined by

$$X_k(g) = X(D_k(g)),$$

we may construct an "inner product"

$$X_2^*X_1 = \text{av}_g\, X_2^*(g)X_1(g)$$

by averaging (integrating) over the group.

[6] C. Chevalley, *Lie Groups*, (Princeton University Press, Princeton, New Jersey, 1946), p. 16.

2. The Determinant

Although, because we used the spectral resolution techniques, there is no primary need for a determinant, one would like to have such a quantity to decide whether a given transformation is regular (i.e., has an inverse) or not.

Here at least as much care is needed as for the character. Clearly the usual definitions of the determinant of a matrix are of no use here because of noncommutativity. The determinant serves to determine the conditions under which two linearly independent vectors remain independent after a given linear transformation. Take, for simplicity, the unit vectors

$$\begin{pmatrix}1\\0\end{pmatrix} \quad \begin{pmatrix}0\\1\end{pmatrix}$$

and the transformation $\begin{pmatrix}a & b\\ c & d\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$ become $\begin{pmatrix}a\\c\end{pmatrix}$ and $\begin{pmatrix}b\\d\end{pmatrix}$, respectively. By definition the question of independence reduces to the question of whether or not

$$a/b = a\cdot b^{-1} \quad \text{equals} \quad c/d = c\cdot d^{-1},$$

i.e., whether or not $ab^{-1} - cd^{-1} = 0$.

In order to get rid of the reciprocals, one might want to multiply this quantity with bd from the right, but then one arrives at $ad - cd^{-1}bd$, and now there is no way to eliminate d^{-1} in the second term. So one is forced to define another concept which will replace the usual determinant. The usual determinant $\Delta(M)$, M = any matrix, is a multiplicative mapping of the full real (complex) matrix ring on the field of real (complex) numbers, i.e., if $C = A\cdot B$ then $\Delta(C) = \Delta(A)\Delta(B)$. Instead of a mapping of the full quaternionic matrix ring on the field of quaternions, we define a "Δ mapping" of this ring on the set of non-negative real numbers. This is accomplished by the following definition:

In the quaternion theory, $\Delta(M)$ shall be the product of all the eigenvalues of M^HM. M^HM is a Hermitian non-negative matrix which, by the spectral theorem of Sec. II has n real eigenvalues ≥ 0. These are all > 0 except when M is singular, in which case one or more of them $= 0$. For nonsingular M, therefore, ln M^HM is defined, and $\Delta(M) = \exp X\ (\ln M^HM)$.

That this determinant is multiplicative is proved by the remark that it reduces to the ordinary determinant in the symplectic picture, which is an isomorphism of the full quaternionic matrix M.

We note that $\Delta(U) = 1$ for every unitary matrix and $\Delta(MNM^{-1}) = \Delta(N)$ if M is nonsingular.

This determinant or Δ mapping provides a criterion for the regularity or singularity of a linear transformation. The circumstance that our definition of the quaternionic determinant $\Delta(M)$ is always positive is unavoidable for it is a homomorphism into an Abelian group. Such an Abelian group is necessarily a subgroup of the factor group of Q over its commutator subgroup, the sphere of quaternions of modulus 1.[7]

Clearly the new trace and the new determinant are a generalization to quaternion matrices of the real part and the norm of quaternion numbers. In analogy to the character $X(M)$, it is possible to give a definition of $\Delta(M)$ which has the same form for all three fields R, C, Q, reproduces the usual concepts for the usual fields R, C, and gives our new determinant in the quaternion case.

3. Schur's Lemma

Let $\{U\}$, $\{U'\}$ be irreducible sets of linear operators on Q spaces V, V'. Let there exist a linear transformation T on V into V' such that the two sets $\{U'T\}$ and $\{TU\}$ (of linear transformations on V into V') contain the same elements:

$$\{U'T\} = \{TU\}.$$

Then either $T = 0$, or dim V = dim V' and T is nonsingular.

Proof: cf. reference 5, (second edition, 1957), p. 237.

Let $S = TV$ be the image of V in V' under T. Then S is invariant under $\{U'\}$: For let Tv be an arbitrary element of S, with v in V, and U' be an arbitrary element of $\{U'\}$; then for some u in $\{U\}$

$$u'Tv = Tuv,$$

which is again in S. Since $\{U'\}$ is irreducible, either $S = 0$ or $S = V'$. If $S = 0$ then $T = 0$, while if $S = V'$ then dim $V' \leq$ dim V. Thus $T = 0$ or dim $V' \leq$ dim V. Now take the Hermitian adjoint of the assumed relation

$$\{U'T\} = \{TU\}.$$

This interchanges the roles of U and U', and replaces T by T^H, so we conclude analogously that either $T^H = 0$ or dim $V \leq$ dim V'. Combining the two results, either $T = 0$ or dim V = dim V'. In the latter case, T is nonsingular. This proves Schur's lemma for Q spaces. As in the complex

[7] We have been informed that the same concept was also introduced by Moore, and called the "norm determinant," see E. H. Moore, Mem. Am. Phil. Soc. 1, 99, 141 (1935).

case, it follows from this lemma that the characters of 2 inequivalent representations are orthogonal.

4. The Corollary to Schur's Lemma

Theorem: If a Hermitian matrix H commutes with an irreducible set D of matrices, it is a (real) multiple of the unit matrix.

Proof: We use the *ersatz* determinant. Since

$$HD = DH,$$
$$\text{and} \qquad ED = DE, \qquad E = \text{the unit matrix},$$

by subtraction $(H - \lambda E)D = D(H - \lambda E)$.

Now,

$$M^+M = (H - \lambda E)^+(H - \lambda E)$$
$$= H^2 - 2\lambda H + \lambda^2 E.$$

H is nonsingular and has real eigenvalues λ_k. Therefore H^2 has eigenvalues λ_k^2.

Since H^2, λH, and $\lambda^2 E$ all commute, we see that M^+M can be made singular by putting $\lambda = \lambda_k$, for then one of the eigenvalues of M^+M becomes $\lambda_k^2 - 2\lambda_k^2 + \lambda_k^2 = 0$, and $\Delta(M) = 0$ whence $M^+M = 0$ and $M = 0$, $H = \lambda E$.

5. The Frobenius-Schur Classification

Frobenius and Schur classified all irreducible C-representations with respect to whether or not they leave invariant a bilinear form.

Assume that a representation D leaves invariant a non-degenerate bilinear form C

$$D^T C D = C$$

or

$$CD = D^A C$$

where $D^A \equiv D^{T-1}$ is the adjoint representation. Taking the adjoint of this equation, multiplying by C from the left and using the very same equation again, we get:

$$C^A D^A = DC^A$$
$$CC^A D^A = CDC^A = D^A CC^A$$

and by the corollary to Schur's lemma: $CC^A = \lambda E$, λ a scalar, that is $C = \lambda C^T$ or else $C \equiv 0$.

Taking the transpose of this equation, $C^T = \lambda C$; and inserting it, we get:

$$C = \lambda C^T = \lambda^2 C,$$

or

$$\lambda = \begin{cases} +1 & C = +C^T \\ 0 & C = 0 \\ -1 & C = -C^T \end{cases}$$

One may therefore say (Frobenius, and Schur, loc. cit.): an irreducible representation belongs to class $+1, 0, -1$ if it leaves invariant a symmetric bilinear form, no bilinear form, or a skew symmetric bilinear (symplectic) form, respectively. For unitary representations this may be expressed also in a different way. The first equation can be written: $CDC^{-1} = D^A$ but if D is unitary $D^A = D^{-1T} = D^*$.

Therefore if D belongs to class $+1$ or to class -1, it is equivalent to the complex conjugate representation and all characters (in the usual complex sense) $X(D)$ are real: if D belongs to class 0, D and D^* are not equivalent. Moreover it can be shown that a $D \in$ class $+1$ is equivalent to a real representation.

6. The Main Reduction Theorem

We now are able to state the main reduction theorem: A representation D, irreducible over C, reduces over Q into two representations $D_1 \oplus D_2$ if and only if $D \in$ class -1. D_1 and D_2 are equivalent and irreducible over Q.

We restrict ourselves to the case where G is compact and $D(G)$ may therefore be assumed unitary, such that $D^A = D^*$. First we prove that the condition $D \in$ class -1 is necessary.

a. Assume $D \in$ class 0, suppose that D reduces over Q. This means that there is a nonsingular (quaternionic) Hermitian operator M such that

$$MD = DM, \qquad M^H = M.$$

We decompose $M = M_0 + M_2$,

$$[M_0, i_3]_- = [M_2, i_3]_+ = 0.$$

Since $i_3 D = D i_3$,

$$M^{i_3} D = DM^{i_3}, \quad \text{where} \quad M^{i_3} \equiv i_3^{-1} M i_3.$$

But $M^{i_3} = M_0 - M_2$ and therefore both M_0 and M_2 commute with D:

$$M_0 D = DM_0 , \tag{0}$$
$$M_2 D = DM_2 . \tag{2}$$

By the corollary to Schur's lemma (valid in the complex case) $M_0 = \lambda E$, where λ is even and real, since $M_0^H = M_0$.

Now form $K \equiv i_1 M_2$; since M_2 is Hermitian and imaginary, it, together with K, is skew symmetric.

$$[K, i_3]_- = i_1 M_2 i_3 - i_3 i_1 M_2$$
$$= i_1 M_2 i_3 + i_1 i_3 M_2 = i_1 M_2 i_3 = 0,$$

i.e., K is a complex (and again by Schur's lemma, a nonsingular) matrix.

But $D = i_1^{-1}D^*i_1$ and from (2) we get:

$$M_2 D = i_1^{-1}D^* i_1 M_2,$$
$$D = K^{-1}D^*K.$$

That is: $D \simeq D^*$: D is equivalent to the complex-conjugate representation, contrary to the assumption. Of course instead of i_1 we could have used any j, $[j, i_3]_+ = 0$, $j^2 = -1$.

b. A short additional remark is sufficient to dispose of the case $D \in$ class $+1$. $C \neq 0$, $C^T = +C$ since for every matrix $M^Q = M_0^* - M_2$ (we can use here the star, since $[M_0, i_3]_- = 0$).

$$M_2^T = M_2^{HQ} = M_2^Q = -M_2$$

(here use is made of $M^H = M$)

$$K^T = -K.$$

But now

$$D = C^{-1}D^*C = C^{-1}KDK^{-1}C = (K^{-1}C)^{-1}D(K^{-1}C)$$

and by Schur's lemma:

$$K^{-1}C = \lambda E$$
$$C = \lambda K,$$

which is impossible, since a symmetric matrix cannot be a multiple of a skew one, unless $\lambda = 0$ which would mean $C = 0$, contrary to the assumption.

c. We now show that the condition $D_2 \in$ class -1 is *sufficient* for the reduction. Assume

$$CD = D^*C \qquad C^T = -C.$$

But $D^* = i_1^{-1}Di_1$ and with $K = i_1C$, $KD = DK$. We note that $K^H = K$, since $K^H = -C^H i_1 = -i_1C^T = i_1C = K$ can be fulfilled with $C^T = -C$. This completes this part of the proof. It remains to show that D reduces into two equivalent representations irreducible over Q, $D = D_1 \oplus D_2$, $D_1 \simeq D_2$. For this purpose it is sufficient to show that $X(D_1) = X(D_2)$.

According to Frobenius and Schur,[3] it is always possible to transform the representation D so that C assumes its normal form

$$C = \begin{pmatrix} & -E \\ E & \end{pmatrix} = \begin{pmatrix} & -1 \\ 1 & \end{pmatrix} \otimes E.$$

The reducible representation D then is brought into the reduced form $\begin{pmatrix} D_1 & \\ & D_2 \end{pmatrix}$ by the same matrix R which diagonalizes $K = i_1C$:

$$R^{-1}DR = \begin{pmatrix} D_1 & \\ & D_2 \end{pmatrix},$$

$$R^{-1}KR = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \otimes E \text{ or } KR = R \otimes \begin{pmatrix} E & \\ & -E \end{pmatrix}.$$

From the second form of the second equation one deduces:

$$R = \begin{pmatrix} a & i_1 a^* \\ i_1 a & a^* \end{pmatrix} \otimes E,$$

where a is a complex number in the imaginary variable i_1, $2|a|^2 = 1$, for K is complex in the imaginary variable i_1, but we can chose a to be $2^{-1/2}$. If we now write $D = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ where $\alpha, \beta, \gamma, \delta$ are complex matrices in the imaginary variable i_3 the first and the fourth quarter of $R^{-1}DR$ are

$$D_1 = 2^{-1/2} \otimes E \cdot (\alpha - i_1\gamma + \beta i_1 - i_1\,\delta i_1) \cdot 2^{-1/2} \otimes E$$

and

$$D_2 = 2^{-1/2} \otimes E \cdot (-i_1\alpha i_1 + \gamma i_1 - i_1\beta + \delta) \cdot 2^{-1/2} \otimes E.$$

Both matrices have evidently the same real part, therefore the same character, whence it follows that they are equivalent.

Finally, D_1 is irreducible over Q. D is nothing but the symplectic picture of D_1; if D_1 were to reduce over Q, then so would D over C.

That the characters are a complete orthogonal system could probably be shown by going through the work of Peter and Weyl and demonstrating that the proofs remain valid if one considers quaternionic instead of complex integral equations. It also follows, however, from the remark that in view of the definition given in Sec. III.2 that the new D_1 has the same character the old D had, and that the system of characters therefore remains the same, up to a factor 2.

After this work was completed we received a preprint from Professor F. J. Dyson, in which this problem is also treated, but with different methods.

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[8] Dr. Iwahori informed us that he had obtained similar results, however, with very different methods.

Uniqueness and Existence of the Solution to the Static London-Maxwell Equations in Two Dimensions*

FAROUK ODEH
International Business Machines Corporation, Thomas J. Watson Research Center, Yorktown Heights, New York
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A theorem is given for the existence and uniqueness of the time-independent solution of the exterior-interior problem associated with determining the distribution of superconducting current, according to the London model, in simply- or doubly-connected two-dimensional regions. The proof of the corresponding theorem in three dimensions is outlined. A discussion is also given of the relationship between two "different" solutions which already exist for rectangular regions.

THE problem of determining the static current distribution in a superconducting element is of importance in many cryogenic devices. Although the solutions to several special problems, according to the London model, have been known for a long time (Van Laue[1]), it seems that only the cylindrical and spherical geometries have been fully treated. In such cases, because of symmetry, one does not need to discuss the effect of the normal region outside the superconductor. The first discussion of an unsymmetrical case seems to be due to Marcus,[2] who considered the case in which the superconducting current flows along the axis of an infinitely long cylinder with a rectangular cross section. The problem was reduced to an integral equation, with an undetermined constant as the inhomogeneous term, which was solved numerically. This same problem has been redone by Culler and Frantz,[3] who solved, again numerically, an exterior-interior problem for Maxwell's and London's equations. The formulations of the problem in references 2 and 3 are quite different. There appears to be no obvious relationship between the two rather similar solutions. Moreover, the exact conditions imposed on the solution at infinity, although they play an important role in determining the solution, are not made clear. In this report we give a precise formulation (Sec. 1) of the general case when there may exist a number of cylinders whose cross sections $\{\Omega_i\}, i = 1, 2, \cdots, n$ are bounded by smooth closed curves $\{L_i\}$ (Fig. 1). A uniqueness theorem and an existence theorem for the solution are given in Sec. 2. The relationship between the present formulation, which was implicitly adopted by Culler and Frantz, and Marcus' formulation is discussed in Sec. 3. It is shown there that the exterior-interior problem is equivalent (in the interior region) to an integral equation that has the same form as Marcus's equation, but whose inhomogeneous term is a definite constant α, which is a determinable function of the cross section(s) only, and which may be equal to zero in some cases. For the case $\alpha \neq 0$, the existence theorem shows that Marcus's procedure[2] gives the same (and therefore unique) solution as the exterior-interior formulation. An example where $\alpha = 0$ is also given. In such a case the inhomogeneous equation in reference 2 will have no solution, but the solution to the homogeneous part would furnish the desired current distribution.

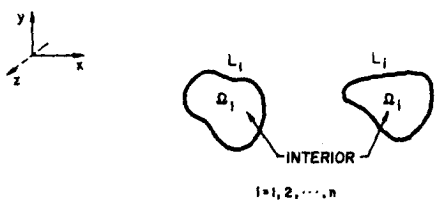

FIG. 1. The interior and exterior regions Ω_i.

1. FORMULATION OF THE PROBLEM

Let $\mathbf{J} = (0, 0, j(x, y))$ be the distribution of current density in $\Omega = \bigcup_i \Omega_i$ and let L^+, L^-, respectively, denote the exterior, interior sides of the boundary $L = \bigcup_i L_i$ (Fig. 2). We assume that the total current flowing in Ω is equal to I. Since $\mathbf{J}$ has a z component only, the magnetic field

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[1] M. Van Laue, *Superconductivity* (Academic Press Inc., New York, 1952).

[2] P. M. Marcus, *Proceedings of the Seventh International Conference on Low Temperature Physics* (University of Toronto Press, Toronto, 1961), pp. 418–421.

[3] G. Culler and L. Frantz, "Current and Magnetic Field Distribution for an Infinitely Long Superconductor of Rectangular Cross-Section," Space Tech. Lab., Report No. 9844-0011-RU-000 and 9844-0025-RU-000 (1961). (Unpublished).

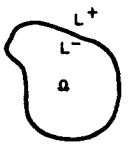

FIG. 2. The interior region Ω and its boundary.

H lies in the x-y plane. The equations to be solved are, therefore

Inside Ω

$$\text{curl } \mathbf{J} = -(1/c\Lambda)\mathbf{H} \quad \text{(London)} \tag{1.1}$$

$$\text{curl } \mathbf{H} = (4\pi/c)\mathbf{J} \quad \text{(Maxwell)} \tag{1.2a}$$

$$\text{div } \mathbf{H} = 0. \quad \text{(Maxwell)} \tag{1.2b}$$

Outside Ω

$$\text{curl } \mathbf{H} = 0$$

$$\text{div } \mathbf{H} = 0. \tag{1.3}$$

The tangential component $\mathbf{H}_t$ of the magnetic field is continuous across L as usual. We assume that the permeability of the exterior and interior materials are equal, and, hence, the normal component of the field $\mathbf{H}_n$, is also continuous, i.e.,

$$\mathbf{H}_t, \mathbf{H}_n \text{ are continuous across } L. \tag{1.4}$$

Introduce now the vector potential **A** via the relationships

$$\text{curl } \mathbf{A} = \mathbf{H} \tag{1.5}$$

$$\text{div } \mathbf{A} = 0. \tag{1.6}$$

The conditions (1.4), (1.5), and (1.6) do not specify **A** completely, since we can add to **A** the gradient of a scalar harmonic function without spoiling them. The potential is determined uniquely in the following manner: By specifying the asymptotic behavior of **A** we determine it up to two additive constants in the outside and the inside regions. The constants are then determined by requiring that the potential is (i) equal to $-c\Lambda\mathbf{J}$ inside Ω, and (ii) is continuous across L. Explicitly, let $\mathbf{A} = (0, 0, \phi(x, y))$ and define

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) - k \ln r, \qquad \mathbf{r} \in \text{exterior} \tag{1.7}$$

where **r** denotes a two-dimensional vector, r is its magnitude, $k = -2I/c$, and the origin of coordinates is taken inside Ω. We further assume that[4,5]

(1) $\psi(\mathbf{r})$ is uniformly bounded,

(2) $r\,\partial\psi/\partial r \to 0$ as $r \to \infty$. (1.8)

Suppose that we wish to add to **A** the gradient $\mathbf{e}u(\mathbf{r})$ of a scalar harmonic function, where **e** is a unit vector in the z direction. Then u would satisfy

$$\nabla^2 u = 0, \qquad \text{outside}$$

$$\nabla^2 u = 0, \qquad \text{inside}, \tag{1.9}$$

and from the continuity of **H** across L

$$\partial u/\partial t,\ \partial u/\partial n \text{ are continuous across } L \tag{1.10}$$

where $\partial/\partial t$, $\partial/\partial n$ denote differentiation along the tangent and the normal to L, respectively. Also

$$u \sim \psi \text{ asymptotically.} \tag{1.11}$$

Using Green's formula, in conjunction with (1.9), (1.10), and (1.11), we get

$$\int_{L^+} u \frac{\partial u^*}{\partial n}\, dl - \int_{L^-} u \frac{\partial u^*}{\partial n}\, dl = \int_E |\nabla u|^2\, dS$$

where dl, dS denote line and area elements, respectively, E denotes the whole space, and u^* is the complex conjugate of u.

Since, from (1.10) $u^+ - u^-$ = a constant c, we then have

$$\int_E |\nabla u|^2\, dS = c \int_L \frac{\partial u^*}{\partial n}\, dl = 0. \tag{1.12}$$

Now, because u is *not* assumed to be continuous in the whole space, Eq. (1.12) implies that u is equal to some constant in Ω and possibly some other constant outside. To fix these constants we define

$$\phi(x, y) = -c\Lambda j(x, y), \qquad (x, y) \in \Omega \tag{1.13}$$

$$\phi \text{ continuous across } L. \tag{1.14}$$

Notice that it is possible to satisfy (1.14) since the values of the potential originally could not have differed across the boundary by more than a constant. The complete problem for ϕ is now restated for further reference: to find a continuous function ϕ which satisfies:

$$\text{(i) } \nabla^2\phi = 0, \qquad \text{outside } \Omega \tag{1.15}$$

$$\text{(ii) } \nabla^2\phi - \beta^2\phi = 0, \quad \text{inside } \Omega \tag{1.16}$$

where $\beta^2 = 4\pi/c^2\Lambda$,

$$\text{(iii) } \phi,\ \partial\phi/\partial n, \quad \text{continuous across } L \tag{1.17}$$

$$\text{(iv) if } \psi(\mathbf{r}) = \phi(\mathbf{r}) - k \ln r,\ \mathbf{r} \in \text{outside} \tag{1.18}$$

[4] The second condition in (1.8) is not necessary in the two-dimensional case since condition (1) implies then, that infinity is a regular point for Laplace's equation, and (2) is then satisfied (see reference 5).

[5] W. Smirnow, *Lehrgang der Höheren Mathematik IV* (Deutsch. Verlag Wissenshaften, Berlin, 1958), pp. 522–525.

where $k = -2I/c$, then $\psi(\mathbf{r})$ is bounded and $r\,\partial\psi/\partial r \to 0$ as $r \to \infty$.

Remark: The procedure used above for producing a continuous vector potential fails in three dimensions if the asymptotic behavior of $\mathbf{A}$ is assumed to be similar to that of a point charge. In fact, if one assumes for that case the continuity of both $\mathbf{A}$ and $\mathbf{H}$, then the only solution to the problem is $\mathbf{A} \equiv 0$ (see Sec. 2).

2. UNIQUENESS AND EXISTENCE OF THE SOLUTION

Uniqueness

Theorem 1: If ϕ is a solution of the problem (1.15), $\cdots$, (1.18), then ϕ is unique.

Proof: Let u be the difference of any two solutions; then u behaves asymptotically like ψ. Applying Green's formula (to the exterior region), we have

$$\lim_{R\to\infty} \int_{\Sigma_R} u \frac{\partial u^*}{\partial r}\, dl = \int_L u \frac{\partial u^*}{\partial n_i}\, dl + \int_{\tilde{\Omega}} |\nabla u|^2\, dS, \quad (2.1)$$

where Σ_R denotes a circle of radius R, n_i and n_e are the interior and exterior normals to L, respectively, and $\tilde{\Omega}$ is the exterior to $\Omega + L$. Also, from Green's formula, in the interior

$$0 = \int_L u \frac{\partial u^*}{\partial n_e}\, dl + \beta^2 \int_\Omega |u|^2\, dS + \int_\Omega |\nabla u|^2\, dS. \quad (2.2)$$

Adding (2.1) and (2.2) we get

$$\lim_{R\to\infty} \int_{\Sigma_R} u \frac{\partial u^*}{\partial r}\, dl = \beta^2 \int_\Omega |u|^2\, dS + \int_E |\nabla u|^2\, dS. \quad (2.3)$$

The left-hand side of (2.3) is equal to zero because of (1.18); hence, the continuity of u implies that u vanishes identically.

Existence

We introduce the following notation:

$G(\mathbf{r}, \mathbf{s}) = \ln|\mathbf{r} - \mathbf{s}|$

B_1 = Banach space of functions continuous on $\Omega + L$, under the maximum norm.

B_2 = Banach space of functions continuous on L, under the maximum norm.

$B = B_1 \otimes B_2 \otimes B_2$, under the maximum of all the norms.

Notice that

$$\nabla^2 G(\mathbf{r}, \mathbf{s}) = -2\pi\, \delta(\mathbf{r} - \mathbf{s}),$$

where $\delta(\mathbf{r})$ is Dirac's delta function.

Instead of working with the vector potential ϕ, it is more convenient to prove the existence of ψ, which, by definition, is

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) - k \ln r, \quad \mathbf{r} \in \text{exterior}$$
$$\psi(\mathbf{r}) = \phi(\mathbf{r}), \quad \mathbf{r} \in \text{interior}.$$

Therefore, ψ is a solution of

$$\nabla^2 \psi = 0. \quad \mathbf{r} \in \text{outside} \quad (2.4)$$

$$(\nabla^2 - \beta^2)\psi = 0, \quad \mathbf{r} \in \text{inside} \quad (2.5)$$

$$\psi^+(\mathbf{r}) - \psi^-(\mathbf{r}) = -k \ln r, \quad \mathbf{r} \in L \quad (2.6)$$

$$\frac{\partial \psi^+}{\partial n} - \frac{\partial \psi^-}{\partial n} = -k \frac{\partial}{\partial n} \ln r, \quad \mathbf{r} \in L \quad (2.7)$$

ψ is bounded and $\partial\psi/\partial r = o(r^{-1})$, at infinity. (2.8)

We seek a representation for ψ, in the interior, in the form of a distribution $\nu(\mathbf{r})$ of poles over Ω together with a different pole distribution $\sigma(\mathbf{r})$ and a dipole distribution $\mu(\mathbf{r})$ over the boundary L. In the outside, the representation is altered slightly to take care of the correct asymptotic behavior of ψ; hence, we want to prove the existence of a vector (ν, σ, μ) which belongs to B such that if $\mathbf{r} \in \Omega$, then

$$\psi(\mathbf{r}) = \int_\Omega G(\mathbf{r}, \mathbf{s})\nu(\mathbf{s})\, dS + \int_L G(\mathbf{r}, \mathbf{s})\sigma(\mathbf{s})\, dl + \int_L \frac{\partial G(\mathbf{r}, \mathbf{s})}{\partial n_s} \mu(\mathbf{s})\, dl. \quad (2.9)$$

while if $\mathbf{r} \in$ exterior, then

$$\psi(\mathbf{r}) = \int_L [G(\mathbf{r}, \mathbf{s}) - (\ln r + f(\mathbf{s}))]\sigma(\mathbf{s})\, dl + \int_L \frac{\partial G(\mathbf{r}, \mathbf{s})}{\partial n_s} \mu(\mathbf{s})\, dl, \quad (2.10)$$

where $f(\mathbf{s}) = (\partial/\partial n_s) \ln s$, $\mathbf{s} \in L$,

and n denotes the exterior normal to Ω. The significance of $f(\mathbf{s})$ and the reason for introducing it will become apparent in the course of the proof. Notice here that if the superconductor consists of more than one cylinder, then both Ω and L in the above equations will denote a collection of disjoint sets. The following analysis remains unchanged. Substituting the representations (2.9) and (2.10) in the problem (2.4), $\cdots$, (2.8), and taking into account the singularities of the line distributions of poles and dipoles, we arrive at the following system of integral equations:

$$0 = 2\pi\nu(\mathbf{r}) + \beta^2\Big[\int_\Omega G(\mathbf{r},\mathbf{s})\nu(\mathbf{s})\,dS + \int_L G\sigma\,dl + \int_L \frac{\partial G}{\partial n_s}\mu\,dl\Big] \qquad \mathbf{r} \in \text{closure of } \Omega \qquad (2.11)$$

$$k\frac{\partial}{\partial n_r}\ln r = 2\pi\sigma(\mathbf{r}) + \int_\Omega \frac{\partial G}{\partial n_s}\nu(\mathbf{s})\,dS + \frac{\partial \ln r}{\partial n_r}\int_L \sigma\,dl, \qquad \mathbf{r} \in L \qquad (2.12)$$

$$-k\ln r = 2\pi\mu(\mathbf{r}) - \int_\Omega G(\mathbf{r},\mathbf{s})\nu(\mathbf{s})\,dS - \int_L [\ln r + f(\mathbf{s})]\sigma\,dl, \qquad \mathbf{r} \in L. \qquad (2.13)$$

Now we have

Lemma 1: The system of equations (2.11), (2.12), and (2.13) have the Fredholm alternative property.[6]

The proof depends on the fact that the 3×3 matrix of integral operators defined by the system is completely continuous on B. This follows from the fact that $G(\mathbf{r}, \mathbf{s})$ is square integrable on both Ω

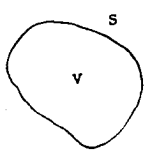

FIG. 3. The three-dimensional region and its boundary.

and L and that $(\partial G/\partial n_s)(\mathbf{r}, \mathbf{s})$ is continuous on L, even at $\mathbf{r} = \mathbf{s}$ (see Riesz and Nagy,[7] Sec. IV). The proof now follows a standard argument.

Lemma 2: The homogeneous system of equations has only the trivial solution.

Proof: Suppose that there exists a vector $\gamma_0 = (\nu_0, \sigma_0, \mu_0)$, which satisfies (2.11), (2.12), and (2.13) with the left-hand side being equal to zero. Define the field $\psi_0(\mathbf{r})$ by using the vector γ_0 in conjunction with (2.9) and (2.10). Then $\psi_0(\mathbf{r})$ will satisfy Eqs. (2.4), $\cdots$, (2.8), but will be continuous and have continuous normal derivatives across L; hence, by the uniqueness theorem, $\psi_0(\mathbf{r}) \equiv 0$. But then, Eq. (2.11) implies that $\nu_0(\mathbf{r}) \equiv 0$, and hence, from (2.12) and (2.13) we get

$$2\pi\sigma_0(\mathbf{r}) = -\frac{\partial \ln r}{\partial n_r}\cdot\gamma \qquad (2.14)$$

$$2\pi\mu_0(\mathbf{r}) = \ln r\cdot\gamma + \int_L f(\mathbf{s})\sigma_0(\mathbf{s})\,dl, \qquad (2.15)$$

where $\gamma = \int \sigma_0\,dl$, $f(\mathbf{s}) = (\partial/\partial n_s)\ln s$.

[6] The existence of the solution to the system follows from the uniqueness of the solution.

[7] F. Riesz and B. Nagy, *Functional Analysis* (Frederick Ungar Publishing Company, New York, 1955).

Substituting these values into (2.11) again (remembering that $\nu_0 \equiv 0$), we get

$$0 = \gamma\int_L\Big[\frac{\partial G(\mathbf{r},\mathbf{s})}{\partial n_s}\ln s - G(\mathbf{r},\mathbf{s})\frac{\partial}{\partial n_s}\ln s\Big]dl + c\int_L \frac{\partial G(\mathbf{r},\mathbf{s})}{\partial n_s}dl, \qquad \mathbf{r} \in \Omega, \qquad (2.16)$$

where

$$c = \int_L f(\mathbf{s})\sigma_0(\mathbf{s})\,dl = -\frac{\gamma}{2\pi}\int_L\Big(\frac{\partial}{\partial n_s}\ln s\Big)^2 dl.$$

Consider the first integral in (2.16). By Green's theorem it is equal to

$$-2\pi\int_\Omega [\ln s\cdot\delta(\mathbf{r}-\mathbf{s}) - \ln|\mathbf{r}-\mathbf{s}|\,\delta(\mathbf{s})]\,dS = 0.$$

Hence the second integral in (2.16) vanishes also, which implies that $c = 0$ and, therefore, $\gamma = 0$. Substituting in (2.14) and (2.15), we get

$$\sigma_0 \equiv \mu_0 \equiv 0,$$

and the assertion of the lemma is proved.

The Fredholm alternative now yields

Theorem 2: There exists a unique solution $\phi(\mathbf{r})$ to the problem (1.15), $\cdots$, (1.18), which is normalized such that $\int_\Omega j(x, y)\,dS = I$.

Proof: Set

$$\phi(\mathbf{r}) = k\ln r + \psi(\mathbf{r}), \quad \mathbf{r} \in \text{outside}$$
$$\phi(\mathbf{r}) = \psi(\mathbf{r}), \quad \mathbf{r} \in \text{inside}$$

where $\psi(\mathbf{r})$ is determined by the unique solution of (2.11), (2.12), and (2.13) and the representations (2.9) and (2.10). It remains only to prove that $\int_\Omega j(x, y)\,dS = I$, but

$$\int_\Omega j(x,y)\,dS = -\frac{1}{c\Lambda}\int_\Omega \phi(x,y)\,dS = -\frac{1}{c\Lambda}\frac{1}{\beta^2}\int_L \frac{\partial\phi}{\partial n}\,dl$$
$$= \lim_{R\to\infty} -\frac{1}{c\Lambda}\frac{c^2\Lambda}{4\pi}\int_{\Sigma_R}\frac{\partial\phi}{\partial r}r\,d\theta = -\frac{c}{4\pi}\Big(-\frac{2I}{c}\Big)2\pi = I.$$

The three-dimensional case

Let V be a superconducting bounded body, and assume its boundary S to be a smooth regular (in the sense of Kellog) surface (or surfaces). In order to determine the static distribution of current inside V we would have to solve the following exterior-interior problem for the vector potential $\mathbf{A}$ (see Fig. 3):

(i) $\nabla \times \nabla \times \mathbf{A} = 0$ outside

(ii) $\nabla \times \nabla \times \mathbf{A} + \beta^2 \mathbf{A} = 0$ inside

(iii) curl $\mathbf{A} = \mathbf{H}$ is continuous across S

and since, at infinity, the potential should behave like that of a point source or a dipole we should have

$$\text{(iv)} \qquad \left.\begin{aligned} \mathbf{A} &= O(1/r) \\ \nabla \times \mathbf{A} &= O(1/r^2) \end{aligned}\right\} \quad \text{as} \quad r \to \infty .$$

We prove now that if $\mathbf{A}$ is assumed to be also continuous across S, then the only solution is $\mathbf{A} \equiv 0$. We begin by a statement of Green's first vector identity.

$$\int_V \mathbf{B} \cdot \nabla \times (\nabla \times \mathbf{C})\, dV - \int_V (\nabla \times \mathbf{B}) \cdot (\nabla \times \mathbf{C})\, dV = \int_S (\nabla \times \mathbf{C}) \times \mathbf{B} \cdot \mathbf{n}\, dS, \qquad (2.17)$$

where $\mathbf{B}$, $\mathbf{C}$, are arbitrary smooth ($C^{(1)}$, $C^{(2)}$, respectively) vectors, and $\mathbf{n}$ is the unit outward normal to S. This formula may be proved by applying the divergence theorem to the vector $\mathbf{B} \times (\nabla \times \mathbf{C})$ and using the identity

$$\nabla \cdot \{\mathbf{B} \times (\nabla \times \mathbf{C})\} = (\nabla \times \mathbf{B}) \cdot (\nabla \times \mathbf{C}) - \mathbf{B} \cdot \nabla \times (\nabla \times \mathbf{C}).$$

Apply (2.17) to the vectors $\mathbf{A}$, $\mathbf{A}^*$ in the region bounded by a large sphere Σ_R and the surface S; then

$$\lim_{R \to \infty} \int_{\Sigma_R} (\nabla \times \mathbf{A}) \times \mathbf{A} \cdot \mathbf{n}\, dS - \int_S (\nabla \times \mathbf{A}) \times \mathbf{A}^* \cdot \mathbf{n}\, dS = -\int_{\text{Outside}} |\nabla \times \mathbf{A}|^2\, dV. \qquad (2.18)$$

Similarly,

$$\int_S (\nabla \times \mathbf{A}) \times \mathbf{A}^* \cdot \mathbf{n}\, dS = -\int_V \beta^2 |\mathbf{A}|^2\, dV - \int_V |\nabla \times \mathbf{A}|^2\, dV. \qquad (2.19)$$

Adding (2.18), (2.19), and using the asymptotic behavior of $\mathbf{A}$ we get

$$\int |\nabla \times \mathbf{A}|^2\, dV + \beta^2 \int_V |\mathbf{A}|^2\, dV = 0.$$

Therefore, $\mathbf{A}$ vanishes identically.

This shows that the vector potential should be discontinuous across the boundary S for the existence of a solution, or that the asymptotic behavior of $\mathbf{A}$ should be altered to $\mathbf{A} = A_0 + O(1/r)$, where A_0 is some nonzero constant. If A_0 is given (or the discontinuity at the surface S is given), then the above argument would show the uniqueness of the potential in such a case. The method of the existence proof generalizes immediately to three dimensions by use of the appropriate Green's function $G(\mathbf{r}, \mathbf{s}) = |\mathbf{r} - \mathbf{s}|^{-1}$.

3. THE ASYMPTOTIC BEHAVIOR OF THE POTENTIAL AND MARCUS' FORMULATION

In the paper by Marcus,[2] the first-order London-Maxwell equations (1.1) and (1.2) were used to arrive at the following integral equation for $\phi(\mathbf{r})$ inside the superconducting region

$$\phi(\mathbf{r}) = C - \frac{\beta^2}{2\pi} \int_\Omega G(\mathbf{r}, \mathbf{s}) \phi(\mathbf{s})\, dS, \qquad \mathbf{r} \in \Omega \qquad (3.1)$$

where C is a constant to be determined by the requirement that $\int_\Omega \phi(\mathbf{r})\, dS = -c\Lambda I$. It is not clear, however, whether the homogeneous version of (3.1) has any solutions or not. If such solutions, i.e., eigenfunctions, exist, then there exists no unique solution to (3.1), or no solution at all depending on the nature of these eigenfunctions. In this section we discuss the relationship between (3.1) and the formulation of Sec. 2. It will be shown that the exterior-interior problem is equivalent, in the interior, to an integral equation, similar in form to (3.1), but which is homogeneous in certain special cases. Hence, the existence and uniqueness theorems of the exterior-interior problem imply that (3.1), for almost all cases, will have a unique solution. In the irregular cases, however, it will have no solutions whatsoever. We now proceed to prove these assertions.

Lemma 3: Let ϕ satisfy the inside-outside problem (1.15), $\cdots$, (1.18); then $\phi(\mathbf{r})$ satisfies the integral equation,

$$2\pi\phi(\mathbf{r}) = 2\pi\alpha - \beta^2 \int_\Omega G(\mathbf{r}, \mathbf{s}) \phi(\mathbf{s})\, dS, \quad \mathbf{r} \in \Omega \qquad (3.1a)$$

where

$$\alpha = \int_L \frac{\partial}{\partial n_s} (\ln s) \sigma(\mathbf{s})\, dl,$$

and $\sigma(\mathbf{s})$ is defined by (2.11), (2.12), and (2.13).

Proof: Let $\mathbf{r}$ be an interior point of Ω. Applying Green's formula in the region Ω to the pair of functions G, ϕ, we get

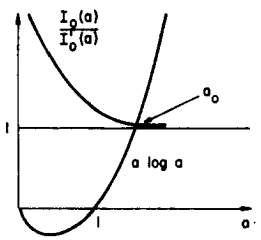

FIG. 4. The radius a_0 of the eigendomain.

$$2\pi\phi(\mathbf{r}) = -\beta^2 \int_\Omega G(\mathbf{r}, \mathbf{s})\phi(\mathbf{s})\, dS + \int_{L^-} \left[G(\mathbf{r}, \mathbf{s}) \frac{\partial \phi}{\partial n} - \phi \frac{\partial G}{\partial n} \right] dl. \qquad (3.2)$$

Let $u(\mathbf{r})$ denote the second integral in (3.2); then, keeping in mind that ϕ is harmonic in the exterior, we have

$$u(\mathbf{r}) = \int_{L^+} [\cdots]\, dl = \lim_{R\to\infty} \times \int_{\Sigma_R} \left[G(\mathbf{r}, \mathbf{s}) \frac{\partial \phi(\mathbf{s})}{\partial s} - \phi(\mathbf{s}) \frac{\partial G}{\partial s} \right] dl.$$

This last integral can be shown to be equal to

$$u(\mathbf{r}) = \lim_{R\to\infty} \int_0^{2\pi} \psi(R, \theta)\, d\theta, \quad \text{independently of } \mathbf{r}.$$

Now the existence theorem, together with the representation (2.10) shows that

$$\psi(\mathbf{r}) = \int_L \frac{\partial}{\partial n_s} (\ln s)\sigma(\mathbf{s})\, dl + O\left(\frac{1}{r}\right), \text{ as } r \to \infty. \qquad (3.3)$$

Therefore, $u(\mathbf{r}) = 2\pi\alpha$ for all $\mathbf{r} \in \Omega$, and the proof is concluded.

The next lemma is obvious.

Lemma 4: Let $\phi_0(\mathbf{r})$ be a solution of (3.1a) for $\mathbf{r} \in \Omega$.[8] Define $\phi(\mathbf{r})$, for all $\mathbf{r}$, by the right side of (3.1a). Then $\phi(\mathbf{r})$ is a solution of the exterior-interior problem (1.15), $\cdots$, (1.18), and ϕ_0 is therefore unique.

The above two lemmas show the equivalence between the exterior-interior problem and the integral equation (3.1a). Hence, the existence and uniqueness theorems of Sec. 2 prove that there exists a unique solution to (3.1a). By comparing (3.1) and (3.1a), we see that the same result holds for Marcus' equation in the case $\alpha \neq 0$. In principle, it is possible to determine whether α vanishes or not by solving the system of equations (2.11), (2.12), and (2.13) and then computing the integral (3.3), which defines α, but this is clearly impractical.

Lemma 5: If $\alpha = 0$, then (3.1) has no solution for any nonzero C.

Proof: Since (3.1) is of the Fredholm type, it is enough to prove that a constant cannot be orthogonal to the solutions of the homogeneous equation. But, if $\alpha = 0$, then Lemma 3 shows that the interior-exterior solution $\phi(\mathbf{r})$ is a solution to the homogeneous equation (3.1). Since Theorem 2 shows that $\int \phi(\mathbf{r})\, dS \neq 0$, the lemma is proved.

An example of the case $\alpha = 0$: The existence of a special case for which $\alpha = 0$ is, by Lemma 3, equivalent to the existence of a certain domain Ω, which makes the quantity $-\beta^2/2\pi$ an eigenvalue of the integral operator $\int_\Omega G(\mathbf{r}, \mathbf{s}) \cdots d\mathbf{s}$. The existence of such a domain follows from the fact that G is symmetric and that the eigenvalues vary continuously with the domain Ω. We shall give now a specific example of such a case.

The representation (2.10) shows that $\phi(\mathbf{r}) = k \ln r + \alpha + O(r^{-1})$ as $r \to \infty$. Let Ω be a circle of radius a and let us seek a radially symmetric solution. If we take $\beta = 1$ for simplicity, then

$$\phi(\mathbf{r}) = k \ln r + \alpha, \qquad \mathbf{r} \in \text{outside}$$

$$\phi(\mathbf{r}) = (k \ln a + \alpha)\, I_0(r)/I_0(a), \qquad \mathbf{r} \in \text{inside}$$

where $I_0(r) \equiv J_0(ir)$ is the Bessel function of the first kind with pure imaginary argument.

The constant α is determined by the continuity of $\partial\phi/\partial r$ at $r = a$, i.e., by the relation

$$k/a = (k \ln a + \alpha) I_0'(a)/I_0(a)$$

or

$$\alpha = k\left[\frac{1}{a}\frac{I_0(a)}{I_0'(a)} - \ln a\right].$$

To make $\alpha = 0$, the radius a should satisfy

$$I_0(a)/I_0'(a) = a \ln a.$$

The last equation has a unique solution a_0 (see Fig. 4). Therefore, if Ω is a circle of radius a_0, then the homogeneous version of (3.1), with $\beta = 1$, will have a solution, ϕ_0, which is unique up to a multiplicative constant, and which determines the current density.

[8] If $\alpha = 0$, then ϕ_0 is chosen such that the right side of (3.1a) is asymptotically equal to $k \ln r$.