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Contraction of Lie Groups*

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Contraction is defined for a Lie group to coincide on its Lie algebra with a generalization of contraction as first introduced by Inönü and Wigner. This is accomplished with a sequence of nonsingular coordinate transformations on the group (or nonsingular linear coordinate transformations on its Lie algebra), whose limit is a singular one. Essentially all of the calculations are performed in the algebra. It is assumed that in the limit the association in the algebra (the multiplication law in the group) converges, and this gives a necessary and sufficient condition on the algebra. Once it is satisfied, the new (contracted) algebra is uniquely determined in terms of the original one. It is found that the contracted algebra can be further contracted in the same way, and likewise the algebra so obtained. In this way one obtains a terminating sequence of algebras. Inönü-Wigner contraction corresponds to a sequence terminating at the first contraction. Some properties of the original and contracted algebras are studied, and some specific examples are given. Contraction of a Lie algebra induces contraction of any of its representations. This is examined for the case of finite-dimensional representations. Ray representations are discussed in general. It is shown how the trivial exponent of the Lorentz group changes under contraction to the nontrivial one of the Galilei group.

INTRODUCTION

THE concept of group contraction was introduced by Inönü and Wigner[1] in a paper which describes some of its general properties and discusses some particular examples. Roughly speaking, their procedure is the following.

Consider a Lie group $G^{(0)}$ and its Lie algebra $\mathfrak{G}^{(0)}$. Assume a coordinate system in $\mathfrak{G}^{(0)}$ in which the elements ξ of the algebra have components ξ^i. Then perform a coordinate transformation in $\mathfrak{G}^{(0)}$ given by

$$\bar{\xi}^i = U_j^i \xi^j,$$

where the matrix U depends on a parameter ε running from some finite value ε_0 to zero. So long as $\varepsilon \neq 0$, U is assumed nonsingular, so that the Lie algebra obtained by the coordinate transformation remains, of course, isomorphic to the original one. If, however, U becomes singular when $\varepsilon = 0$ one may, as IW show, obtain a new Lie algebra (and hence a new Lie group) which is not isomorphic to the original one.

IW find the necessary and sufficient condition that a group can be contracted, assuming that by a suitable choice of nonsingular matrices α and β the matrix U can be transformed to the form

$$\beta U \alpha^{-1} = u + \varepsilon w, \tag{1}$$

where

$$u = \begin{vmatrix} \mathbf{I} & 0 \\ 0 & 0 \end{vmatrix}$$

and

$$w = \begin{vmatrix} v & 0 \\ 0 & \mathbf{I} \end{vmatrix}.$$

In what follows we shall call group contraction so defined [i.e., assuming U can be put in the form of (1)] Inönü-Wigner contraction (or merely IW contraction).

The present purpose is to generalize somewhat this

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[1] E. Inönü and E. P. Wigner, Proc. Natl. Acad. Sci. U. S. **39**, 510 (1953) (hereafter referred to as IW).

concept of group contraction. The motivation is closely related to that of IW. It is essentially physical, and arises from the way in which the Lorentz group contracts to the Galilei group. With this in mind, let us consider a particularly simple example: the inhomogeneous Lorentz group in one timelike and one spacelike dimension. The three parameters v, y, and τ, the velocity of the moving frame, the space translation, and the time translation, define the group elements, which we shall write in the form $\langle v,y,\tau\rangle_\lambda$; here the subscript $\lambda=1/c$ indicates the fact that the group product depends on λ. This product is

$$\langle v_2,y_2,\tau_2\rangle_\lambda\langle v_1,y_1,\tau_1\rangle_\lambda = \left\langle \frac{v_1+v_2}{1+\lambda^2 v_1 v_2},\ y_2+g_2(\lambda)(y_1+v_2\tau_1),\ \tau_2+g_2(\lambda)(\tau_1+v_2 y_1\lambda^2)\right\rangle_\lambda, \quad (2)$$

where $g_2(\lambda)=(1-\lambda^2 v_2^2)^{-\frac{1}{2}}$.

Let us now let c increase without bound, or go to the limit as $\lambda\to 0$. Then (2) becomes

$$\langle v_2,y_2,\tau_2\rangle_0\langle v_1,y_1,\tau_1\rangle_0=\langle v_1+v_2,\ y_1+y_2+v_2\tau_1,\ \tau_2+\tau_1\rangle_0 \quad (3)$$

which is the multiplication law for the Galilei group.

Now this same result could be obtained by considering (2) for $\lambda=1$ and reparametrizing the group so obtained. In particular we may write

$$(v,y,\tau)_\lambda=\langle \lambda v,\lambda y,\tau\rangle_1, \quad (4)$$

and we then find that $(v,y,\tau)_\lambda$ satisfy the same multiplication law as $\langle v,y,\tau\rangle_\lambda$, and in the limit this will also lead to (3). So long as $\lambda\neq 0$, however, it is clear that we have merely performed a coordinate transformation in the original group, which does not change the group in any essential way. When we pass to the limit, on the other hand, the group changes, and this new group is what is called the contracted one.

It might perhaps have been more natural to write, instead of (4),

$$(v,y,\tau)_\lambda=\langle \lambda v,y,\tau/\lambda\rangle_1.$$

This would correspond to writing out the transformations themselves for the variables x and ct rather than x and t, whereas Eq. (4) corresponds to writing out the transformations for x/c and t. Clearly, there is no essential difference between these two schemes. We wish, however, to express the reparametrization linearly in λ, and we therefore choose (4) over the alternate form. It is interesting that this choice of linearity in λ, as is seen from the previous example, is not as restrictive as it seems at first. The degree to which it is restrictive depends to a large extent on the structure of the group.

It is seen from this example that by a suitable reparametrization which is then allowed to tend to a limiting form it is possible to obtain one group from another (though not always one which is not isomorphic). In what follows we generalize the concept of contraction using the previous example as a model.

This paper is divided into two parts. In the first the fundamental results are derived and some examples are given. The second is a discussion of some aspects of representations.

I

A. Contraction

1. Definition

Consider an n-dimensional connected Lie group $G^{(0)}$ and a differentiable coordinate system[2] in it, in which the coordinates of any $x\in G^{(0)}$ are x^i, and the coordinates of the identity e all vanish. Further, consider a sequence of other differentiable coordinate systems, in which the coordinates of x are $\bar{x}^i$ (again we arrange it so that the coordinates of e all vanish). Let these systems be related to the original one by a set of differentiable functions

$$x^i=\varphi^i(\bar{x}^1,\cdots\bar{x}^n,\lambda),$$

depending on a parameter $\lambda(0\leq\lambda\leq 1)$, such that

$$\begin{aligned}\varphi^i(0,\cdots 0,\lambda)&=0,\\ \varphi^i(\bar{x}^1,\cdots,\bar{x}^n,1)&=\bar{x}^i,\end{aligned} \quad (5)$$

and such that the determinant of the

$$U_j{}^i=\left.\frac{\partial\varphi^i}{\partial\bar{x}^j}\right|_{\bar{x}^1=\bar{x}^2=\cdots=\bar{x}^n=0} \quad (6)$$

vanishes if and only if $\lambda=0$, and let the φ^i and their derivatives converge as λ tends to zero. Let the group operation in terms of the unbarred coordinates be

$$(xy)^i=z^i(x^1,\cdots,x^n;y^1,\cdots,y^n)=z^i(x,y), \quad (7)$$

and in the barred system let the coordinates of the product be

$$\bar{z}^i=(\bar{x}^1,\cdots,\bar{x}^n;\bar{y}^1,\cdots,\bar{y}^n)=\bar{z}^i(x,y). \quad (8)$$

It is a simple matter to obtain the $\bar{z}^i$ in terms of the z^i and the set of functions inverse to the φ^i (which exist by assumption for $\lambda\neq 0$).

Thus from the coordinate transformation and the multiplication law in the unbarred coordinates, we can obtain the multiplication law in the barred coordinates. But this will have meaning only if $\lambda>0$, for the functions inverse to the φ^i are not defined at $\lambda=0$. We shall assume, however, that the expression on the right of (8) has a limit as $\lambda\to 0$, which we shall call $z^{(1)i}(x,y)$. This new set of functions defines, in general, a new multiplication law, and hence a new group $G^{(1)}$, which we shall call the *contraction* of $G^{(0)}$. Note that the assumption of the existence of the limit

[2] L. Pontrjagin, *Topological Groups* (Princeton University Press, Princeton, New Jersey, 1946).

is just the assumption that $G^{(0)}$ can be contracted in this way. Our task shall be to find the conditions under which this limit exists and the ensuing consequences.

2. *Lie Algebra*

As is often the case when dealing with Lie groups, it is convenient to pass to the Lie algebra. We wish therefore to restate the assumption that the

$$z^{(1)i}(x,y)=\lim_{\lambda\to 0}\bar{z}^i(x,y) \tag{9}$$

exist in terms of the algebra.

We start by associating in a well-known way[2] with $G^{(0)}$ the n-dimensional vector space S of tangent vectors at the unit element to the curves $x(t)$. The original coordinate system in $G^{(0)}$ induces a coordinate system in S, and in this coordinate system $\xi\epsilon S$ has components $\xi^i(i=1,\cdots,n)$. Under a coordinate transformation given by the φ^i in $G^{(0)}$ the coordinates of ξ change according to [see (6)]

$$\xi^i=U_j{}^i\bar{\xi}^i.$$

The Lie algebra $\mathfrak{G}^{(0)}$ is given by S together with a composition law derived from the multiplication law in $G^{(0)}$. With every pair of vectors ξ, η in S we associate a third vector ζ whose components are

$$\zeta^i=c_{jk}{}^i\xi^j\eta^k, \tag{10}$$

where the $c_{jk}{}^i$ are the well-known structure constants of the group $G^{(0)}$. This equation corresponds to (7) in that the association is induced in the algebra by the multiplication law of the group (and conversely, the so-called covering group can be constructed from the algebra). Now under a coordinate transformation the vector ζ associated with given ξ and η will, of course, not change, though its components will. Thus the $c_{jk}{}^i$ must change, and if we write the new components of ζ in the form

$$\bar{\zeta}^i=\bar{c}_{jk}{}^i\bar{\xi}^j\bar{\eta}^k, \tag{11a}$$

the $c_{jk}{}^i$ are given by the obvious tensor transformation law

$$\bar{c}_{jk}{}^i=(U^{-1})_l{}^i c_{mn}{}^l U_j{}^m U_k{}^n. \tag{11b}$$

These last two equations bear the same relation to (8) as (10) does to (7). Clearly Eq. (11b) is meaningless when $\lambda=0$, for U^{-1} is then not defined. But we have assumed that as $\lambda\to 0$ the $\bar{z}^i\to z^{(1)i}$. As λ varies, we can obtain the $\bar{c}_{jk}{}^i$ in the usual way from the $\bar{z}^i$, and these are given by (11b). In particular, in the limit $\lambda=0$ the $z^{(1)i}$ give limiting values for the structure constants, and these define the Lie algebra of the contracted group (the contracted algebra). Thus if the $\bar{z}^i$ have a limit, so do the $\bar{c}_{jk}{}^i$.

Conversely, if (11b) has a limit as λ tends to zero, the multiplication law defined by the $\bar{c}_{jk}{}^i$ will have a limit. Further, the limit obtained by constructing the multiplication law from the $\bar{c}_{jk}{}^i$ and then letting λ tend to zero is the same as that obtained by constructing the multiplication law from the limiting structure constants (see Appendix). Thus we see that so long as we are interested in a small enough region about the unit element, the Lie algebra is sufficient for our purposes.

Let us restate our results somewhat, taking the "active" rather than "passive" view of the transformation. We shall write the association in a coordinate-system independent form: with every ξ and η in S we associate a ζ according to

$$\zeta=[\xi,\eta].$$

This bracket has all of its well-known properties: it is antisymmetric, linear, and satisfies the Jacobi identity. Further, the $U_j{}^i$ now will define a mapping rather than a coordinate transformation. In other words, the vector $\bar{\xi}$ with components $\bar{\xi}^i$ is mapped by U into $\xi=U\bar{\xi}$, with components $\xi^i=U_j{}^i\bar{\xi}^j$. In the process the bracket must change, so that if $\zeta=[\xi,\eta]$, then $\bar{\zeta}=[\bar{\xi},\bar{\eta}]'$ (the prime denotes that the bracket is not the same one as before the mapping; it is, in fact, λ-dependent). This is evidently a restatement of (11a) and (11b). We are now interested in how the bracket changes under the mapping. Accordingly, we consider

$$\bar{\zeta}=[\bar{\xi},\bar{\eta}]'=U^{-1}\zeta=U^{-1}[\xi,\eta]=U^{-1}[U\bar{\xi},U\bar{\eta}]. \tag{12}$$

Going to the limit, we find that the Lie algebra $\mathfrak{G}^{(1)}$ of the contracted group is given by

$$[\xi,\eta]^{(1)}=\lim_{\lambda\to 0}U(\lambda)^{-1}[U(\lambda)\xi,U(\lambda)\eta] \tag{13}$$

(the bars have been dropped and the λ-dependence of U indicated).

Thus we study the contraction of a (local) Lie group by studying the contraction of its Lie algebra according to (13).

3. *Necessary and Sufficient Condition for Contraction. The bracket in* $\mathfrak{G}^{(1)}$

Note that U was defined [see Eq. (6)] so that $U(1)=\mathbf{I}$. This is not necessary, but involves no loss of generality, since a nonsingular coordinate transformation in $G^{(0)}$ can always be made to bring this about. As was mentioned in the Introduction, we shall consider only $U(\lambda)$ linear in λ. Then we write

$$\begin{aligned}U(\lambda)&=u+\lambda w\\&=\lambda\mathbf{I}+(1-\lambda)u.\end{aligned}$$

From the condition that $U(\lambda)$ is singular if and only if $\lambda=0$, it follows that $U(0)=u$ is singular. With this expression for $U(\lambda)$, Eq. (12) becomes [here $\mu=\lambda/(1-\lambda)$]

$$[\xi,\eta]'=\{1/(\mu+1)\}(\mu+u)^{-1}[(\mu+u)\xi,(\mu+u)\eta]. \tag{14}$$

Note that the limit as $\lambda \to 0$ is the same as the limit as $\mu \to 0$.

Equation (14) contains the inverse of $(\mu+u)$, and this inverse exists by assumption so long as $\mu \neq 0$. We proceed to find it as follows. Let S_R and S_N be subspaces of S such that

$$u^n S = S_R$$
$$u^n S_N = 0.$$

(Here n is the dimension of S. The last equation is meant in the sense that S_N is the maximum space annihilated by u^n, or $u^n\xi = 0$ if and only if $\xi \epsilon S_N$.) From these definitions it follows[3] that S_N and S_R reduce u, and that u is nonsingular when restricted to S_R and nilpotent when restricted to S_N. Further,

$$S_N \oplus S_R = S.$$

Since S_R is invariant under u, and u is nonsingular on S_R, there is no problem in defining an inverse for u on S_R, and we shall call it simply u^{-1}. For convenience (to make clear what happens in the limit) we write

$$(\mu+u)^{-1} = u^{-1}(\mu u^{-1}+\mathbf{1})^{-1} \quad \text{on} \quad S_R.$$

Further, it is easily verified that

$$(\mu+u)^{-1} = -\frac{1}{\mu}\sum_{j=0}^{q-1}\left(-\frac{u}{\mu}\right)^j \quad \text{on} \quad S_N,$$

where q is the lowest power of u which annihilates S_N.

Since in the limit as $\mu \to 0$ the factor $1/(1+\mu) \to 1$, we shall drop it from our discussion of (14). Then except for this factor (14) becomes, when expanded in powers of μ,

$$[\xi,\eta]' = (\mu+u)^{-1}\{\mu^2[\xi,\eta]+\mu([u\xi,\eta]+[\xi,u\eta]) + [u\xi,u\eta]\}. \quad (15)$$

We break up the brackets into their projections into S_R and S_N, writing

$$\sigma = \sigma_R+\sigma_N = [\xi,\eta]$$
$$\tau = \tau_R+\tau_N = [u\xi,\eta]+[\xi,u\eta]$$
$$\pi = \pi_R+\pi_N = [u\xi,u\eta],$$

where for any vector $\zeta \epsilon S$ we write

$$\zeta = \zeta_R+\zeta_N,\ \zeta_R \epsilon S_R,\ \zeta_N \epsilon S_N.$$

(These projections into S_R and S_N are unique.) Then (15) becomes

$$[\xi,\eta]' = u^{-1}(\mu u^{-1}+\mathbf{1})^{-1}(\mu^2\sigma_R+\mu\tau_R+\pi_R) + \frac{1}{\mu}\sum_{j=0}^{q-1}\left(\frac{-u}{\mu}\right)^j(\mu^2\sigma_N+\mu\tau_N+\pi_N).$$

In this limit as $\mu \to 0$ this becomes

$$[\xi,\eta]' = u^{-1}\pi_R - u\sigma_N+\tau_N+\lim_{\mu\to 0} \times\left(\frac{1}{\mu}-\frac{u}{\mu^2}+\cdots\right)(u^2\sigma_N-u\tau_N+\pi_N). \quad (16)$$

If this is to converge as $\mu \to 0$, then we must demand that

$$u^2\sigma_N+u\tau_N+\pi_N = 0,$$

or

$$u^2[\xi,\eta]_N - u[u\xi,\eta]_N - u[\xi,u\eta]_N + [u\xi,u\eta]_N = 0. \quad (17)$$

This is the necessary and sufficient condition that $G^{(0)}$ can be contracted with the given φ^i (or U), stated in terms of the Lie algebra $\mathfrak{G}^{(0)}$ and $u = U(0)$. That it depends only on $U(0)$ follows from our choice $U(1) = 1$ and the linear λ-dependence of $U(\lambda)$.

It will be convenient to rewrite (17) in another form. By applying $u^{r-2}(r = 2,3,\cdots)$ to (17), we have

$$u^r[\xi,\eta]_N - u^{r-1}[\xi,u\eta]_N = u^{r-1}[u\xi,\eta]_N - u^{r-2}[u\xi,u\eta]_N.$$

This equation is satisfied for all $r > 1$ and all ξ and η, so we may use it to reduce the power of u (if $r > 2$) operating on the brackets on the right. This means we can move factors of u one at a time from outside the brackets into the brackets (operating on the first vector in the brackets). In this way we arrive eventually at

$$u^r[\xi,\eta]_N - u^{r-1}[\xi,u\eta]_N = u[u^{r-1}\xi,\eta]_N - [u^{r-1}\xi,u\eta]_N. \quad (17a)$$

Note that this equation is valid for $r = 1,2,\cdots$ (for $r = 1$ it is an identity), and is entirely equivalent to (17).

Now if (17) is satisfied we may go to the limit $\mu = 0$ in (16) [recalling (13)]

$$[\xi,\eta]^{(1)} = u^{-1}[u\xi,u\eta]_R - u[\xi,\eta]_N + [u\xi,\eta]_N + [\xi,u\eta]_N. \quad (18)$$

This is the defining equation for $\mathfrak{G}^{(1)}$, the contracted Lie algebra. (Note again that u^{-1} is defined only on S_R.) We will say that contracting $\mathfrak{G}^{(0)}$ by u gives $\mathfrak{G}^{(1)}$.

B. Sequence of Contracted Algebras

1. *Structure of* $\mathfrak{G}^{(0)}$

Equation (17) is a requirement on $\mathfrak{G}^{(0)}$. From it we may deduce the following.

Lemma 1. If u contracts $\mathfrak{G}^{(0)}$ [satisfies (17)], then so does $u^m (m = 1,2,\cdots)$.

Proof. We remark first that the equations

$$(u^m)^n S_N = 0$$
$$(u^m)^n S = S_R$$

[3] P. R. Halmos, *Finite Dimensional Vector Spaces* (Princeton University Press, Princeton, New Jersey, 1948).

define the same subspaces of S as did the similar equations in which u^m was replaced by u. Thus we may make use of the projections into these subspaces.

In order to prove the lemma we show that (17a) is satisfied if u is replaced everywhere by u^m. We thus consider (dropping the subscript N on the brackets)

$$I=u^{mr}[\xi,\eta]-u^{m(r-1)}[\xi,u^m\eta].$$

We factor $u^{m(r-1)-1}$ from this expression,[4] and in (17a) we write $r=m+1$ and interchange the vectors in the brackets. It is then seen that

$$\begin{aligned}I&=u^{m(r-1)-1}\{u^{m+1}[\xi,\eta]-u[\xi,u^m\eta]\}\\&=u^{m(r-1)-1}\{u^m[u\xi,\eta]-[u\xi,u^m\eta]\}\\&=u^{mr-1}[u\xi,\eta]-u^{m(r-1)-1}[u\xi,u^m\eta].\end{aligned}$$

This expression for I can be obtained from the previous one by moving one factor of u from outside the brackets onto ξ in the brackets. On repeating this procedure for a total of $m(r-1)$ times, we arrive at

$$\begin{aligned}I=u^{mr}[\xi,\eta]-u^{m(r-1)}[\xi,u^m\eta]\\=u^m[u^{m(r-1)}\xi,\eta]-[u^{m(r-1)}\xi,u^m\eta].\end{aligned}$$

But this is just (17a) with u replaced by u^m, which proves the lemma.

We may use (17) also to prove the following proposition concerning the structure of $\mathfrak{G}^{(0)}$.

Lemma 2. The subspace uS of S forms a subalgebra in $\mathfrak{G}^{(0)}$.

Proof. Let ξ' and η' be in uS. Then there exist ξ and η in S such that $\xi'=u\xi$ and $\eta'=u\eta$. Now according to (17)

$$[u\xi,u\eta]_N=-u(u[\xi,\eta]_N-[u\xi,\eta]_N-[\xi,u\eta]_N),$$

which is obviously in uS. Further $S_R\subset uS$, so that $[u\xi,u\eta]_R\epsilon uS$. Since

$$[u\xi,u\eta]_N+[u\xi,u\eta]_R=[u\xi,u\eta]=[\xi',\eta'],$$

we see that

$$[\xi',\eta']\epsilon uS.$$

This proves the lemma.

Corollary. The subspace u^mS of S (with $m=1,2,\cdots$) forms a subalgebra in $\mathfrak{G}^{(0)}$. In particular this is true of $S_R=u^nS$.

This follows immediately from lemma 1.

2. Contraction of $\mathfrak{G}^{(1)}$

We will show now that $\mathfrak{G}^{(1)}$ can also be contracted by u by showing that (17) is satisfied when $[\xi,\eta]$ is replaced by $[\xi,\eta]^{(1)}$. As in lemma 1, the significance of S_R and S_N remains the same, and we may continue to use their properties. In other words, the subscripts N and R have the same value when discussing the bracket in $\mathfrak{G}^{(1)}$ and in $\mathfrak{G}^{(0)}$.

[4] We need consider only $r>1$, since otherwise (17a) is an identity even if u is replaced by u^m. Also, we are interested only in $m>1$. Therefore all exponents appearing in the proof are positive.

Let us then calculate (again dropping the subscript N)

$$J=u^2[\xi,\eta]^{(1)}-u[u\xi,\eta]^{(1)}-u[\xi,u\eta]^{(1)}+[u\xi,u\eta]^{(1)}.$$

We use (18) [dropping the first term, for (17) involves only the projections into S_N], obtaining

$$\begin{aligned}J=&-u^3[\xi,\eta]+2u^2([u\xi,\eta]+[\xi,u\eta])-u([u^2\xi,\eta]\\&+[\xi,u^2\eta]+3[u\xi,u\eta])+[u^2\xi,u\eta]+[u\xi,u^2\eta]\\&=-uf(\xi,\eta)+f(u\xi,\eta)+f(\xi,u\eta)=0,\end{aligned}$$

where we have written $f(\xi,\eta)$ for the vanishing function of ξ and η given by (17).

Thus $\mathfrak{G}^{(1)}$ can be contracted by u, which means that lemmas 1 and 2 and the corollary to 2 hold for $\mathfrak{G}^{(1)}$ as well as for $\mathfrak{G}^{(0)}$. Let us call $\mathfrak{G}^{(2)}$ the algebra obtained when $\mathfrak{G}^{(1)}$ is contracted by u.

3. Sequence of Contracted Algebras

We are led in this way to a sequence of algebras each of which is obtained from the previous one by contraction by u. That $\mathfrak{G}^{(2)}$ can be contracted by u follows from the fact that $\mathfrak{G}^{(1)}$ can; we call the algebra so obtained $\mathfrak{G}^{(3)}$. In this way we form the sequence, writing symbolically

$$\mathfrak{G}^{(i+1)}=u\cdot\mathfrak{G}^{(i)},$$

where $v\cdot\mathfrak{G}$ is the algebra obtained when a given algebra $\mathfrak{G}$ is contracted by a given singular matrix v. We will now show that all the $\mathfrak{G}^{(i)}$ of the sequence are related as follows.

Lemma 3. $u^i\cdot\mathfrak{G}^{(j)}=\mathfrak{G}^{(i+j)}$.

Proof. First note that it is sufficient to prove the lemma for $j=0$. Indeed, we may start a sequence with any $\mathfrak{G}^{(j)}$, $j=0, 1, \cdots$, so that from this point of view $\mathfrak{G}^{(0)}$ plays no special role.

The proof proceeds by induction. The lemma holds by definition for $i=1$ (and $j=0$). Assume it true for $i=s$. Then the bracket in $\mathfrak{G}^{(s+1)}=u\cdot\mathfrak{G}^{(s)}$ is given by

$$\begin{aligned}[\xi,\eta]^{(s+1)}=&u^{-1}[u\xi,u\eta]_R{}^{(s)}-u[\xi,\eta]_N{}^{(s)}\\&+[u\xi,\eta]_N{}^{(s)}+[\xi,u\eta]_N{}^{(s)}\\=&u^{-(s+1)}[u^{s+1}\xi,u^{s+1}\eta]_R+u^{s+1}[\xi,\eta]_N\\&-u[u^s\xi,\eta]_N-u[\xi,u^s\eta]_N-u^s[u\xi,\eta]_N\\&+[u^{s+1}\xi,\eta]_N+[u\xi,u^s\eta]_N-u^s[\xi,u\eta]_N\\&+[u^s\xi,u\eta]_N+[\xi,u^{s+1}\eta]_N.\end{aligned}$$

The bracket in $u^{s+1}\cdot\mathfrak{G}^{(0)}$ is

$$\begin{aligned}A=&u^{-(s+1)}[u^{s+1}\xi,u^{s+1}\eta]_R-u^{s+1}[\xi,\eta]_N\\&+[u^{s+1}\xi,\eta]_N+[\xi,u^{s+1}\eta]_N.\end{aligned}$$

The S_R projections of these two brackets are the same. Thus the difference between them lies entirely in S_N and is (dropping the subscript N)

$$\begin{aligned}&[\xi,\eta]^{(s+1)}-A\\&=u^{s+1}[\xi,\eta]-u^s[\xi,u\eta]-u[u^s\xi,\eta]+[u^s\xi,u\eta]\\&\quad+u^{s+1}[\xi,\eta]-u^s[u\xi,\eta]-u[\xi,u^s\eta]+[u\xi,u^s\eta],\end{aligned}$$

which vanishes according to (17a). Therefore

$$A=[\xi,\eta]^{(s+1)},$$

which proves the assertion.

It will be seen later that the sequence we have defined is finite in the sense that after a certain algebra (which is, in fact $\mathfrak{G}^{(q)}$, where q is the lowest power of u which annihilates S_N) further contraction gives only isomorphic algebras. The proof of this depends on some properties of the contracted algebras, to which we now turn.

4. *Properties of the* $\mathfrak{G}^{(i)}$

We remark first that lemmas 1 and 2 apply to every $\mathfrak{G}^{(i)}$ of the sequence. In particular, for instance, u^iS forms a subalgebra in each of the $\mathfrak{G}^{(i)}$. There follow some further structural properties of the $\mathfrak{G}^{(i)}$.

(a) Let S_i be the null space of u^i, i.e., $\xi\epsilon S_i$ if and only if $u^i\xi=0$. Then S_i forms an ideal in $\mathfrak{G}^{(i+j)}$, $j=0,1,\cdots$. Recall that an ideal (or normal subalgebra) $\mathfrak{A}$ of a Lie algebra $\mathfrak{G}$ is a subalgebra for which $\xi\epsilon\mathfrak{A}$ implies that $[\xi,\eta]\epsilon\mathfrak{A}$ for all $\eta\epsilon\mathfrak{G}$. It is the Lie algebra of a normal subgroup of the Lie group.

We first prove the assertion for $i=1$, $i+j=m\geq 1$. Assume $\xi\epsilon S_1$. Then in $\mathfrak{G}^{(i+j)}=\mathfrak{G}^{(m)}$ the bracket is

$$[\xi,\eta]^{(m)}=u^{-1}[u\xi,u\eta]_R{}^{(m-1)}-u[\xi,\eta]_N{}^{(m-1)}+[u\xi,\eta]_N{}^{(m-1)}+[\xi,u\eta]_N{}^{(m-1)}.$$

The first and third terms vanish because $u\xi=0$. Then

$$u[\xi,\eta]^{(m)}=-u^2[\xi,\eta]_N{}^{(m-1)}+u[\xi,u\eta]_N{}^{(m-1)}=-u[u\xi,\eta]_N{}^{(m-1)}+[u\xi,u\eta]_N{}^{(m-1)},$$

where we have used (17) as applied to $\mathfrak{G}^{(m-1)}$. This last expression vanishes because $u\xi=0$. Thus $u[\xi,\eta]^{(m)}=0$, or $[\xi,\eta]^{(m)}\epsilon S_1$, as asserted. Now we can replace u by u^i in this proof so long as $m-i\geq 0$. Hence the assertion is true for any i.

What this means is that S_1 forms an ideal in $\mathfrak{G}^{(1)}$; S_1 and S_2 form ideals in $\mathfrak{G}^{(2)}$; S_1, S_2, and S_3 form ideals in $\mathfrak{G}^{(3)}$; etc.

(b) Let $\mathfrak{G}_j{}^{(i)}$ be the ideal formed by S_j in $\mathfrak{G}^{(i)}$ (with $j\leq i$). Then the derived algebra of $\mathfrak{G}_m{}^{(m+l)}$ is contained in S_{m-l} (where we call $S_0=S_{-1}=\cdots=0$). Recall that the derived algebra $\mathfrak{G}'$ of a Lie algebra $\mathfrak{G}$ is made up of all linear combinations of elements of the form $[\xi,\eta]$, where ξ and η are in $\mathfrak{G}$.

To prove this assertion, let $\xi,\eta\epsilon S_m$. Then

$$[\xi,\eta]^{(m+l)}=u^{-l}[u^l\xi,u^l\eta]_R{}^{(m)}-u^l[\xi,\eta]_N{}^{(m)}+[u^l\xi,\eta]_N{}^{(m)}+[\xi,u^l\eta]_N{}^{(m)}.$$

Since ξ and η are annihilated by u^m, so are $u^l\xi$ and $u^l\eta$, which are thus in S_m. But S_m forms an ideal in $\mathfrak{G}^{(m)}$, so that $[u^l\xi,u^l\eta]^{(m)}\epsilon S_m$. It is clear, however, that $S_m\bigcap S_R=0$, for nothing in S_R is annihilated by any power of u. Thus the first term vanishes. The second term is in S_{m-l}, for $[\xi,\eta]_N{}^{(m)}\epsilon S_m$, and if $\zeta\epsilon S_m$, then $u^l\zeta\epsilon S_{m-l}$ (for $u^{m-l}(u^l\zeta)=u^m\zeta=0$). Finally, each of the last two terms is in S_{m-l}; for $u^l\xi$, for instance, is in S_{m-l}, and this forms an ideal in $\mathfrak{G}^{(m)}$. A moment's thought will show that these statements are true whether l is less than, equal to, or greater than m. Since each of the terms in the decomposition of $[\xi,\eta]^{(m+l)}$ is in S_{m-l}, so is $[\xi,\eta]^{(m+l)}$ itself. This proves the assertion.

Note that it follows that $\mathfrak{G}_m{}^{(2m+j)}$ $(j=0,1,\cdots)$ is an *Abelian* Lie algebra (an Abelian ideal in $\mathfrak{G}^{(2m+j)}$). For example, S_1 forms an Abelian ideal in $\mathfrak{G}^{(2)}$, $\mathfrak{G}^{(3)}$, $\cdots$; S_2 forms an Abelian ideal in $\mathfrak{G}^{(4)}$, $\mathfrak{G}^{(5)}$, $\cdots$.

(c) We see from the foregoing that no algebras of the sequence past $\mathfrak{G}^{(0)}$ are simple; all have ideals. Further, none past $\mathfrak{G}^{(1)}$ are semisimple: all have solvable (in fact Abelian) ideals.[5] We will see now that $\mathfrak{G}^{(1)}$ is not semisimple. In fact $\mathfrak{G}_1{}^{(1)}$ is solvable.

In proving this we shall need to make use of the relation

$$S_1\bigcap u^iS=u^iS_{i+1},$$

which we prove first. Let $\xi\epsilon(S_1\bigcap u^iS)$. Then there exists an $\eta\epsilon S$ such that $u^i\eta=\xi$. But $u^{i+1}\eta=u\xi=0$, so that $\eta\epsilon S_{i+1}$, and $\xi\epsilon u^iS_{i+1}$. Conversely let $\xi\epsilon u^iS_{i+1}$. Then clearly $\xi\epsilon u^iS$. Further, $u\xi\epsilon u^{i+1}S_{i+1}=0$, so that ξ is in S_1 and hence also in $S_1\bigcap u^iS_{i+1}$. This proves the relation.

Now let ξ and η be vectors in S_1. For such vectors (18) reduces to

$$[\xi,\eta]^{(1)}=-u[\xi,\eta]_N.$$

Since $\mathfrak{G}_1{}^{(1)}$ is an ideal this bracket is in S_1, and it is obviously in uS. Thus the derived algebra of $\mathfrak{G}_1{}^{(1)}$ is in $S_1\bigcap uS=uS_2$. Now consider $\xi,\eta\epsilon uS_2$. Since uS is a subalgebra in $\mathfrak{G}^{(0)}$, it follows that $u[\xi,\eta]_N\epsilon u^2S$. Thus $[\xi,\eta]^{(1)}\epsilon S_1\bigcap u^2S=u^2S_3$, or the derived algebra of the algebra formed by uS_2 in $\mathfrak{G}^{(1)}$ is in u^2S_3. Proceeding by induction, consider $\xi,\eta\epsilon u^iS_{i+1}$. Since u^iS is a subalgebra in $\mathfrak{G}^{(0)}$, it follows that $u[\xi,\eta]_N\epsilon u^{i+1}S$. Thus

$$[\xi,\eta]^{(1)}\epsilon S_1\bigcap u^{i+1}S=u^{i+1}S_{i+2}.$$

We proceed in this way until we come to $\xi,\eta\epsilon S_1\bigcap u^{q-1}S=u^{q-1}S_q$ (note that $S_q=S_N$ by definition). For these ξ,η, the bracket $[\xi,\eta]^{(1)}$ is in $S_1\bigcap u^qS=S_1\bigcap S_R=0$. Thus this bracket vanishes, and $\mathfrak{G}_1{}^{(1)}$ is solvable.

(d) Recall that S_R forms a subalgebra in every algebra of the sequence. These subalgebras are all isomorphic. This is easily shown if we recall that two Lie algebras $\mathfrak{G}$ and $\mathfrak{G}'$ are isomorphic if there exists a one-to-one mapping A of $\mathfrak{G}$ onto $\mathfrak{G}'$ such that for all $\xi,\eta\epsilon\mathfrak{G}$

$$[\xi,\eta]=A^{-1}[A\xi,A\eta]'. \tag{19}$$

Here $[\ \ ]$ is the bracket in $\mathfrak{G}$, and $[\ \ ]'$ is the bracket in $\mathfrak{G}'$.

[5] A simple Lie algebra has no ideals. A semisimple one has no solvable ideals. Solvable may be defined as follows: Let $\mathfrak{G}'$ be the derived algebra of $\mathfrak{G}$, $\mathfrak{G}''$ the derived algebra of $\mathfrak{G}'$, etc. Then $\mathfrak{G}$ is solvable if the sequence $\mathfrak{G}$, $\mathfrak{G}'$, $\mathfrak{G}''$, $\cdots$ terminates with zero.

With this in mind, we consider $\xi,\eta\epsilon S_R$. Then for any m Eq. (18) becomes

$$[\xi,\eta]^{(m)}=u^{-m}[u^m\xi,u^m\eta],$$

for S_R forms a subalgebra in $\mathfrak{G}^{(0)}$. Thus we see that the algebras formed by S_R in the $\mathfrak{G}^{(m)}$ are all isomorphic to that in $\mathfrak{G}^{(0)}$, and hence to each other.

Other properties of the $\mathfrak{G}^{(i)}$ can be deduced from (17) and (18), but since they are of questionable value, we will not list them here.

(e) Finally, we show that the sequence terminates with $\mathfrak{G}^{(q)}$. More specifically, $\mathfrak{G}^{(q)}$ is isomorphic to $\mathfrak{G}^{(q+j)}$, $j=0, 1, \cdots$.[6]

Consider $\xi,\eta\epsilon S_N$. Then $u^q\xi=u^q\eta=0$. For such vectors, then, (18) gives

$$[\xi,\eta]^{(q+j)}=-u^{q+j}[\xi,\eta]_N=0, j=0, 1, \cdots.$$

Now consider $\xi\epsilon S_N$, $\eta\epsilon S_R$. Then (18) gives

$$\begin{aligned}[\xi,\eta]^{(q+j)}&=-u^{q+j}[\xi,\eta]_N+[\xi,u^{q+j}\eta]_N\\&=[\xi,u^{q+j}\eta]_N,\quad j=0, 1, \cdots.\end{aligned}$$

Finally, consider $\xi,\eta\epsilon S_R$. Then

$$[\xi,\eta]^{(q+j)}=u^{-(q+j)}[u^{q+j}\xi,u^{q+j}\eta],\quad j=0, 1, \cdots.$$

Now let us define a mapping A_j of S on itself by

$$\begin{aligned}A_j\xi&=\xi \quad \text{if} \quad \xi\epsilon S_N,\\A_j\xi&=u^j\xi \quad \text{if} \quad \xi\epsilon S_R.\end{aligned}$$

It is seen that A is nonsingular. Then

$$[\xi,\eta]^{(q+j)}=A_j^{-1}[A_j\xi,A_j\eta]^{(q)}\quad j=0, 1, \cdots,$$

as is easily verified from the foregoing. Therefore all the $\mathfrak{G}^{(q+j)}$ are isomorphic to $\mathfrak{G}^{(q)}$ (and hence to each other).

5. *Summary*

Let us collect the results of Secs. I and II. The notation, where unexplained, has been explained in the foregoing.

Theorem. Let $G^{(0)}$ be an n-dimensional Lie group, and let the differentiable functions $\varphi^i(x^1,\cdots,x^n;\lambda)$ define a coordinate transformation in $G^{(0)}$ which becomes singular in the limit as $\lambda\rightarrow 0$, where the φ^i have the properties indicated in Eq. (5). Then in this limit we obtain a new group, in general not isomorphic to $G^{(0)}$, called the contracted group $G^{(1)}$, if and only if Eq. (17) is satisfied in the Lie algebra $\mathfrak{G}^{(0)}$ of $G^{(0)}$. The Lie algebra $\mathfrak{G}^{(1)}$ of $G^{(1)}$ is given by (18). Further contraction by u (the same coordinate transformation) leads to a sequence of algebras $\mathfrak{G}^{(i)}$, where $\mathfrak{G}^{(i+1)}$ is obtained by contracting $\mathfrak{G}^{(i)}$ by u. Any algebra in the sequence can be obtained from any previous one by contraction by a power of u; i.e., $\mathfrak{G}^{(i+j)}$ can be obtained by contracting $\mathfrak{G}^{(i)}$ by u^j. This sequence terminates at least with $\mathfrak{G}^{(q)}$, where q is the least integer for which $u^qS=u^nS$. In every algebra of the sequence the u^iS form subalgebras. The subalgebras formed by u^nS in each of the $\mathfrak{G}^{(i)}$ are isomorphic. If S_i is the null space of u^i for some i, then it forms an ideal in $\mathfrak{G}^{(i+j)}$, $=0, 1, \cdots$. The only algebra of the sequence that may be simple or semisimple is $\mathfrak{G}^{(0)}$.

We now turn to a discussion of the relation between IW contraction and the more general kind defined here, and to several examples.

C. IW Contraction. Examples

1. *Case $q=1$*

We will show that IW contraction is for us the special case $q=1$. For this case

$$uS=S_R,\quad uS_N=0. \tag{20}$$

Equivalently, as we will show, we may write

$$uS\bigcap S_1=0. \tag{21}$$

It is clear that (20) implies (21) (since $S_N=S_q=S_1$ in this case). That the converse is also true is seen as follows. Assume there exists a $\xi\epsilon S$ such that $u^i\xi=0$ with $i>1$. Then clearly $u^{i-1}\xi=\eta$ is in uS. Further, $u\eta=u^i\xi=0$, so that $\eta\epsilon S_1$, and $\eta=0$ by (21). In other words, if $u^i\xi=0$, all lower positive powers of u, including u itself, annihilate ξ. Thus $u^nS_N=0$ implies that $uS_N=0$, and hence (20) follows from (21).

What will be demonstrated, therefore, is that the IW case corresponds to Eq. (21), and thus to $q=1$. Temporarily we shall use IW notation.

Clearly we may set $\varepsilon_0=1$, say by dividing through by ε_0, after which ε becomes what we have called λ. Now let us subject the I_ν to the transformation

$$\beta=\begin{vmatrix}(1+v)^{-1} & 0\\ 0 & 1\end{vmatrix}.$$

That $(1+v)^{-1}$ exists we know, for when $\varepsilon=1$ the matrix

$$U_\nu{}^i|_{\varepsilon=1}:\begin{vmatrix}(1+v) & 0\\ 0 & 1\end{vmatrix}$$

is nonsingular by assumption. Then u and w take on the forms

$$u=\begin{vmatrix}(1+v)^{-1} & 0\\ 0 & 0\end{vmatrix};\quad w=\begin{vmatrix}(1+v)^{-1}v & 0\\ 0 & 1\end{vmatrix}. \tag{22}$$

When $\varepsilon=1$, the matrix $U_\nu{}^i$ now becomes the unit matrix. The situation is now the same as ours, except that what we call λ, IW call ε.

It is clear that with u in this form Eq. (21) is satisfied. Thus IW contraction leads to $q=1$. To prove that $q=1$ leads to IW contraction, we proceed as follows.

[6] This is not the same statement as IW's assertion that if a group is contracted twice with respect to the same subgroup, the second contraction is without effect. In our terms this means, as we shall see later, tht $\mathfrak{G}^{(2q)}$ is isomorphic to $\mathfrak{G}^{(q)}$.

Consider a vector $\xi \epsilon S_R$. It is clear that $u\xi \epsilon S_R$, and hence that

$$w\xi = (\mathbf{I}-u)\xi = \xi - u\xi \epsilon S_R.$$

Thus not only u, but also w maps S_R into itself. Since u has an inverse on S_R, we may define

$$v = u^{-1} - \mathbf{I} \quad \text{on} \quad S_R.$$

Then

$$\left.\begin{aligned} u &= (\mathbf{I}+v)^{-1} \\ w &= (\mathbf{I}+v)^{-1}v \end{aligned}\right\} \quad \text{on} \quad S_R. \tag{23}$$

Let us turn to S_N. For all $\xi \epsilon S_N$ we have $u\xi = 0$, so that

$$U(1)\xi = (u+w)\xi = \mathbf{I}\xi = w\xi.$$

Thus

$$\left.\begin{aligned} u &= 0 \\ w &= \mathbf{I} \end{aligned}\right\} \quad \text{on} \quad S_N. \tag{24}$$

Equations (23) and (24) put u and w into the form of (22), which completes the proof.

Another way to characterize IW contraction[7] is by the way U^{-1} depends on λ. In IW contraction this dependence is linear in $1/\lambda$. For higher q higher powers of $1/\lambda$ enter U^{-1}.

Consider a general (not IW) contraction by u^q, which we shall call Q. We see that

$$QS = S_R, \quad QS_N = 0,$$

which is just (20) with u replaced by Q. Thus this contraction is an IW contraction. The algebra $\mathfrak{G}^{(q)}$ on which our sequence terminates, therefore, can be obtained from $\mathfrak{G}^{(0)}$ by a single IW contraction by $Q = u^q$.

Finally, we remark without proof that in the IW case Eq. (17) is entirely equivalent to the requirement that S_R form a subalgebra in $\mathfrak{G}^{(0)}$ (corresponding, in IW terminology, to the subgroup of $G^{(0)}$ with respect to which one contracts).

2. *Property of IW Contraction*

One other property of IW contraction will be found useful later. This is that the contracted algebra is completely defined (up to an isomorphism) when S_R is specified. The choice of S_R does not determine S_N uniquely, but any choice of S_N such that $S_N \oplus S_R = S$ will lead to the same (isomorphic) algebra.

More rigorously, let u and v be two mappings leading to IW contraction such that

$$uS = vS = S_R, \quad uS_N = 0, \quad vS_M = 0,$$

for which the null spaces are unequal: $S_N \neq S_M$ (it is nevertheless true, of course, that $S_R \oplus S_N = S_R \oplus S_M = S$).

[7] I am indebted to Professor Wigner for pointing out this fact.

Then as we have seen, S_R forms a subalgebra in $\mathfrak{G}^{(0)}$, and we obtain two contracted algebras defined by

$$\mathfrak{G}^{(u)}: [\xi,\eta]^{(u)} = u^{-1}[u\xi,u\eta]_R + [u\xi,\eta]_N + [\xi,u\eta]_N$$
$$\mathfrak{G}^{(v)}: [\xi,\eta]^{(v)} = v^{-1}[v\xi,v\eta]_R + [v\xi,\eta]_M + [\xi,v\eta]_M$$

for all $\xi,\eta \epsilon S$.

Then $\mathfrak{G}^{(u)}$ is isomorphic to $\mathfrak{G}^{(v)}$.

Proof. Let E and F be projection operators defined, respectively, by the decompositions $S = S_R \oplus S_N$ and $S = S_R \oplus S_M$. In other words,

$$ES = S_R \qquad FS = S_R$$
$$ES_N = 0 \qquad FS_M = 0$$
$$E^2 = E = FE \qquad F^2 = F = EF.$$

Now consider

$$A = u^{-1}vF + (\mathbf{I}-E)(\mathbf{I}-F)$$

(u^{-1} is defined, for the purposes of this expression, by its action on S_R). It is easily seen that A maps S_R onto itself in a one-to-one way and that it maps S_M onto S_N, annihilating nothing. The inverse of A is

$$A^{-1} = v^{-1}uE + (\mathbf{I}-F)(\mathbf{I}-E).$$

We will show that

$$A[\xi,\eta]^{(v)} = [A\xi,A\eta]^{(u)} \tag{25}$$

for all $\xi,\eta \epsilon S$, which is then proof that $\mathfrak{G}^{(u)}$ and $\mathfrak{G}^{(v)}$ are isomorphic.

First let $\xi,\eta \epsilon S_M$. Then $[\xi,\eta]^{(v)} = 0$, and the left side of (25) vanishes. The right-hand side vanishes because $A\xi$ and $A\eta$ are in S_N.

Second, let $\xi,\eta \epsilon S_R$. Then

$$\begin{aligned} A[\xi,\eta]^{(v)} &= Av^{-1}[v\xi,v\eta]_R = u^{-1}vv^{-1}F[vF\xi,vF\eta]_R \\ &= u^{-1}[uA\xi,uA\eta]_R = [A\xi,A\eta]^{(u)}. \end{aligned}$$

Here we have used the fact that $F\zeta = \zeta$ for all ζ in S_R, as well as that $A\xi$ and $A\eta$ are in S_R.

Finally, let $\xi \epsilon S_R$, $\eta \epsilon S_M$. Then using the fact that $A\zeta = (\mathbf{I}-E)\zeta$ for $\zeta \epsilon S_M$, we have

$$\begin{aligned} A[\xi,\eta]^{(v)} &= A[v\xi,\eta]_M = (\mathbf{I}-E)[uA\xi,\, E\eta + (\mathbf{I}-E)\eta]_M \\ &= [uA\xi,E\eta]_N + [uA\xi,\, (\mathbf{I}-E)\eta]_N. \end{aligned}$$

The first of these terms vanishes, for $uA\xi$ and $E\eta$ are both in S_R. As for the second, because $\eta \epsilon S_M$ we may write

$$(\mathbf{I}-E)\eta = (\mathbf{I}-E)(\mathbf{I}-F)\eta = A\eta,$$

and this is in S_N, so that

$$A[\xi,\eta]^{(v)} = [uA\xi,A\eta]_N = [A\xi,A\eta]^{(u)}.$$

Thus (25) is verified for all $\xi,\eta \epsilon S$, and the assertion is proved.

We now turn to some examples of contractions.

3. Three-Dimensional Homogeneous Lorentz Group

Consider the group of homogeneous Lorentz transformations in two spacelike and one timelike dimensions. For physical reasons this group is usually contracted to the corresponding Galilei group. This is an IW contraction with a two-dimensional S_1 (corresponding to the two velocity components). Thus S_R is one-dimensional (corresponding to rotations in space). But this Lorentz group has two-dimensional subgroups (its Lie algebra has two-dimensional subalgebras), so that it can be contracted with a two-dimensional uS, and it is not necessary that $uS=S_R$. Let us therefore contract the group with a two-dimensional uS, although this would seem to have no physical significance.

Since $\dim(uS)=2$ is the rank of u, and $\dim S_1$ is the nullity of u, we see that $\dim S_1=1$. Then $\dim S_R$ may be two, one, or zero ($S_R=0$). We will classify the contractions by $\dim S_R$.

The Lie algebra $\mathfrak{G}^{(0)}$ of the three-dimensional homogeneous Lorentz group can be characterized by the fact that its derived algebra is three-dimensional and that it contains a two-dimensional subalgebra.[8] We need not make use of this second property specifically, since it will follow from the choice of nullity of u and the use of (17), which together guarantee that uS be two-dimensional and that it form a subalgebra in $\mathfrak{G}^{(0)}$. Making use of the first property and the well-known Jacobi identity, we can write the algebra quite generally in the form

$$\begin{aligned}[\alpha_1,\alpha_2]&=r_0\alpha_0+r_1\alpha_1+r_2\alpha_2\\ [\alpha_2,\alpha_0]&=r_1\alpha_0+s_1\alpha_1+s_2\alpha_2\\ [\alpha_0,\alpha_1]&=r_2\alpha_0+s_2\alpha_1+t_2\alpha_2,\end{aligned}\tag{26}$$

where α_0, α_1, and α_2 span S, and the determinant

$$\Delta=\begin{vmatrix} r_0 & r_1 & r_2\\ r_1 & s_1 & s_2\\ r_2 & s_2 & t_2\end{vmatrix}\neq 0.\tag{27}$$

We will treat only one of the three cases in detail. The other results are obtained similarly, and the details will be found in D.

First consider $\dim S_R=0$. Since $u^3S=S_R=0$, we have $S_3=S$. Then it is easily seen that $\dim S_2=2$ (remember that $\dim S_1=1$ by assumption). We choose in S vectors α_0, α_1, α_2 such that

$$\begin{aligned}u\alpha_0&=0 \quad (\alpha_0 \text{ spans } S_1)\\ u\alpha_1&=\alpha_0 \quad (\alpha_0 \text{ and } \alpha_1 \text{ span } S_2)\\ u\alpha_2&=\alpha_1 \quad (\alpha_0,\ \alpha_1, \text{ and } \alpha_2 \text{ span } S_3=S).\end{aligned}\tag{28}$$

[8] V. Bargmann (private communication).

Equations (28) are invariant under the transformation

$$\begin{aligned}\alpha_0'&=\lambda\alpha_0\\ \alpha_1'&=\lambda\alpha_1+\mu\alpha_0\\ \alpha_2'&=\lambda\alpha_2+\mu\alpha_1+\nu\alpha_0,\end{aligned}\tag{29}$$

where λ, μ, and ν are numbers.

Now consider $\xi=\alpha_0$ and $\eta=\alpha_1$ in (17). We have, noting that $S_N=S$ for this case,

$$u^2(r_2\alpha_0+s_2\alpha_1+t_2\alpha_2)=t_2\alpha_0=0,$$

so that

$$t_2=0.$$

Similarly, $\xi=\alpha_2$ and $\eta=\alpha_0$ gives

$$s_2=0,$$

and $\xi=\alpha_1$, $\eta=\alpha_2$ gives

$$s_1=-2r_2.$$

By using these relations we may rewrite (26), and then with this and (18) we obtain the bracket in $\mathfrak{G}^{(1)}$. The results are

$$\begin{aligned}[\alpha_1,\alpha_2]&=r_0\alpha_0+r_1\alpha_1+r_2\alpha_2 & [\alpha_1,\alpha_2]^{(1)}&=2r_1\alpha_0-r_2\alpha_1\\ [\alpha_2,\alpha_0]&=r_1\alpha_0-2r_2\alpha_1 & [\alpha_2,\alpha_0]^{(1)}&=-r_2\alpha_0\\ [\alpha_0,\alpha_1]&=r_2\alpha_0 & [\alpha_0,\alpha_1]^{(1)}&=0.\end{aligned}$$

According to Eq. (27), $\Delta=2(r_2)^3\neq 0$, so that we may write

$$\lambda=-\frac{1}{r_2},\quad \mu=\frac{r_1}{(r_2)^2},\quad \nu=-\frac{1}{(r_2)^2}\left[\frac{r_0}{2}+\frac{(r_1)^2}{r_2}\right],$$

and insert these expressions into (29). Then for the α_i' we have (dropping the primes)

$$\begin{aligned}[\alpha_1,\alpha_2]&=-\alpha_2 & [\alpha_1,\alpha_2]^{(1)}&=\alpha_1,\\ [\alpha_2,\alpha_0]&=2\alpha_1 & [\alpha_2,\alpha_0]^{(1)}&=\alpha_0,\\ [\alpha_0,\alpha_1]&=-\alpha_0 & [\alpha_0,\alpha_1]^{(1)}&=0.\end{aligned}\tag{30}$$

This was the case with $q=3$. The cases with $\dim S_R=1$ ($q=2$) and $\dim S_R=2$ (IW contraction) are handled similarly.

The three contracted algebras so obtained turn out to be isomorphic. Since $q=1$ in the case of a two-dimensional S_R, all the contractions of the three-dimensional Lorentz group are equivalent to IW contraction in the sense that the contracted algebra is always isomorphic to one obtained by IW contraction. One must be careful, however, in speaking of equivalent results. A given vector may play different roles in different contracted algebras. For instance, for $\dim S_R=1$, the vectors whose $\mathfrak{G}^{(1)}$ brackets are given by the second half of (30) have $\mathfrak{G}^{(0)}$ brackets of the form, for instance,

$$\begin{aligned}[\alpha_1,\alpha_2]&=-\alpha_2\\ [\alpha_2,\alpha_0]&=k\alpha_1+\alpha_2\\ [\alpha_0,\alpha_1]&=-\alpha_0+\alpha_1,\end{aligned}\tag{31}$$

where k is an arbitrary nonzero number (it depends on the exact form of u). These brackets are clearly not the same as those in the first half of (30), and thus involve different vectors. Particularly if physical significance is to be attached to general contraction, such differences may be important.

Finally, it is interesting to complete the sequence of contractions in both cases where this is possible.

For $\dim S_R=0$, using (30), we obtain

$$\begin{aligned}&\mathfrak{G}^{(2)}:\ [\alpha_1,\alpha_2]^{(2)}=-2\alpha_0,\quad [\alpha_2,\alpha_0]^{(2)}=[\alpha_0,\alpha_1]^{(2)}=0\\&\mathfrak{G}^{(3)}:\qquad [\alpha_i,\alpha_j]^{(3)}=0\quad i,j=0,1,2.\end{aligned}\tag{32}$$

For $\dim S_R=1$ we obtain

$$\mathfrak{G}^{(2)}:\ [\alpha_i,\alpha_j]^{(2)}=0.$$

For $\dim S_R=2$, the contraction is IW, so there is only $\mathfrak{G}^{(1)}$. It can be shown also that all these are equivalent to others obtained by IW contraction from $\mathfrak{G}^{(0)}$ (of course $\mathfrak{G}^{(3)}$ of the first case and $\mathfrak{G}^{(2)}$ of the second are in fact obtained by IW contraction of $\mathfrak{G}^{(0)}$ by u^3 and u^2, respectively).

The $\mathfrak{G}^{(1)}$ we have obtained is the Lie algebra of the inhomogeneous Lorentz group in one timelike and one spacelike dimension.

4. *Property of the Three-Dimensional Rotation Group*

Before going on to demonstrate a case of general contraction equivalent to no IW contraction, we show that the three-dimensional rotation group can be contracted in only one way (except for the trivial contraction).[9] This contraction is IW contraction, and $\mathfrak{G}^{(1)}$ is the Lie algebra of the Euclidean motions in the plane.

Proof. The Lie algebra of the three-dimensional rotation group can be characterized by the fact that its derived algebra is three-dimensional and it has no two-dimensional subalgebras.[8] We wish to find all possible u's by which this Lie algebra $\mathfrak{G}^{(0)}$ can be contracted.

First, since uS forms a subalgebra in $\mathfrak{G}^{(0)}$ (and the rank of u is less than $\dim S=3$), $\dim(uS)$ must be 1 or 0. We will not consider $\dim(uS)=0$; this is the trivial contraction. Thus $\dim(uS)=1$. Since $S_R\subseteq uS$, it follows that $\dim S_R\leq 1$.

The case $\dim S_R=1$ is just the IW contraction to the Euclidean motions (this contraction is discussed by IW), for then $S_R=uS$, so that $q=1$. We wish to show that it is impossible to contract with $\dim S_R=0$.

If $S_R=0$, then $q=2$. Indeed, let uS (of dimension 1 by assumption) be spanned by a vector η. Then $u=0$, for (1) $u\eta\epsilon uS$, and (2) $u\eta\neq k\eta$ with $k\neq 0$, or S_R would not be empty. Thus for any $\xi\epsilon S$ we have $u^2\xi=u(r\eta)=ru\eta=0$, where r is some constant, so that $u^2S=0$.

[9] We call the trivial contraction the (IW) contraction with $u=0$. Every group can be so contracted, and the result is the n-dimensional Abelian group.

Now it is a well-known fact that the Lie algebra of the three-dimensional rotation group can be represented by ordinary vector-space with the cross product defining the bracket. It is clear also from what has been said about u previously that there exist three linearly independent unit vectors $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$, $\boldsymbol{\alpha}_3$ such that

$$\begin{aligned}&u\boldsymbol{\alpha}_1=r\boldsymbol{\alpha}_2\\&u\boldsymbol{\alpha}_2=u\boldsymbol{\alpha}_3=0.\end{aligned}\tag{33}$$

Since $\boldsymbol{\alpha}_2$ and $\boldsymbol{\alpha}_3$ span a two-dimensional subspace, we may choose them as orthogonal unit vectors. Let $\boldsymbol{\alpha}_1'=\boldsymbol{\alpha}_2\times\boldsymbol{\alpha}_3$. Then writing $\boldsymbol{\alpha}_1'=\rho_1\boldsymbol{\alpha}_1+\rho_2\boldsymbol{\alpha}_2+\rho_3\boldsymbol{\alpha}_3$, we see that we may choose $\boldsymbol{\alpha}_1$ equal to $\boldsymbol{\alpha}_1'$, for $\boldsymbol{\alpha}_2$ and $\boldsymbol{\alpha}_3$ do not contribute to $u\boldsymbol{\alpha}_1'$ (ρ_1 can be absorbed in r). Thus $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$, $\boldsymbol{\alpha}_3$ may be taken as an orthonormal basis. We now check (17). On putting $\xi=\boldsymbol{\alpha}_1$, $\eta=\boldsymbol{\alpha}_3$, we have

$$\begin{aligned}u(u\boldsymbol{\alpha}_1\times\boldsymbol{\alpha}_3)+u(\boldsymbol{\alpha}_1\times u\boldsymbol{\alpha}_3)-u\boldsymbol{\alpha}_1\times u\boldsymbol{\alpha}_3\\=u(\boldsymbol{\alpha}_2\times\boldsymbol{\alpha}_3)=u\boldsymbol{\alpha}_1=r\boldsymbol{\alpha}_2=0.\end{aligned}\tag{34}$$

Thus $r=0$, or $u=0$ and the contraction is the trivial one.

We see here an example of the way in which (17) eliminates what may seem at first a possible contraction. As will be discussed later, the group theoretical or Lie-algebra meaning of (17) is not entirely clear.

5. *Example of a General Contraction Equivalent to No IW Contractions*

The last two paragraphs give examples in which either IW contraction alone is possible or in which any contraction is equivalent to IW contraction. We now give an example of a more general contraction.

Consider the four-dimensional Lie algebra $\mathfrak{G}^{(0)}$ defined by

$$\begin{aligned}&[\alpha_1,\alpha_2]=\alpha_3,\quad [\alpha_2,\alpha_3]=\alpha_1,\quad [\alpha_3,\alpha_1]=\alpha_2,\\&[\alpha_i,\alpha_0]=0.\end{aligned}\tag{35}$$

Here the first three equations give the Lie algebra $\mathfrak{R}_3$ of the three-dimensional rotation group. The algebra $\mathfrak{G}^{(0)}$ is the direct sum of $\mathfrak{R}_3$ and the one-dimensional algebra spanned by α_0. We shall contract this by the mapping u defined by

$$u\alpha_1=u\alpha_2=0,\quad u\alpha_3=\beta=\alpha_0+\alpha_3,\quad u\beta=0.\tag{36}$$

It will be convenient to deal with $\mathfrak{G}^{(0)}$ in terms of α_1, α_2, α_3, and β (rather than α_0). We remark therefore that $\mathfrak{G}^{(0)}$ may be defined by

$$\begin{aligned}&\mathfrak{R}_3\\&[\beta,\alpha_1]=\alpha_2,\quad [\beta,\alpha_2]=-\alpha_1,\quad [\beta,\alpha_3]=0,\end{aligned}\tag{35'}$$

where by $\mathfrak{R}_3$ we mean just the first three equations of (35).

To see that u will indeed give a contraction of $\mathfrak{G}^{(0)}$ we note that $S_R=0$ and $q=2$ (so that $u^2=0$). Then (17) becomes

$$u[u\xi,\eta]+u[\xi,u\eta]-[u\xi,u\eta]=0.$$

Now uS is one-dimensional, so the last term vanishes. Further, uS is spanned by β, and $[\beta,\zeta]$ is a linear combination of α_1 and α_2 for all ζ. Since $u\alpha_1=u\alpha_2=0$, the first two terms vanish separately, and hence (17) is satisfied.

Again recalling that $S_R=0$, Eq. (18) becomes

$$[\xi,\eta]^{(1)}=-u[\xi,\eta]+[u\xi,\eta]+[\xi,u\eta].$$

Then using (36) we obtain

$$\begin{aligned}&[\alpha_1,\alpha_2]^{(1)}=-\beta\\&[\alpha_2,\alpha_3]^{(1)}=\alpha_1\\&[\alpha_3,\alpha_1]^{(1)}=\alpha_2\\&[\beta,\alpha_i]^{(1)}=0\qquad(i=1,2,3),\end{aligned}\tag{37}$$

which defines $\mathfrak{G}^{(1)}$.

Incidentally, further contraction by the same u leads to the four-dimensional Abelian algebra, as is obvious from the fact that $S_R=0$ and $q=2$, so contraction by u^2 is trivial.

We will now show that this result cannot be obtained by IW contraction of $\mathfrak{G}^{(0)}$. Although this can be proven differently (see Appendix II of D), we will do it by performing all possible IW contractions on $\mathfrak{G}^{(0)}$. In the present case this is quite easy because the structure of $\mathfrak{G}^{(0)}$ is particularly convenient.

First, every two-dimensional subalgebra of $\mathfrak{G}^{(0)}$ is spanned by α_0 and some $\rho\epsilon\mathfrak{R}_3$. Indeed, let $\mathfrak{A}_2$ be a two-dimensional subalgebra. Then $\dim(\mathfrak{A}_2\bigcap\mathfrak{R}_3)$ is clearly either one or two (zero is impossible, since $\dim(\mathfrak{A}_2+\mathfrak{R}_3)$ is at most $\dim\mathfrak{G}^{(0)}=4$). As the intersection of two Lie algebras is itself a Lie algebra, $\mathfrak{A}_2\bigcap\mathfrak{R}_3$ must be a subalgebra of $\mathfrak{R}_3$. But $\mathfrak{R}_3$ has no two-dimensional subalgebras. Thus $\dim(\mathfrak{A}_2\bigcap\mathfrak{R}_3)=1$. Let this intersection be spanned by some $\rho\epsilon\mathfrak{R}_3$, and let $\mathfrak{A}_2$ be spanned by ρ and $\alpha_0+\sigma$, where $\sigma\epsilon\mathfrak{R}_3$. Then since $\mathfrak{A}_2$ is a subalgebra,

$$[\alpha_0+\sigma,\rho]=[\sigma,\rho]=r\rho,$$

where r is some number. Thus σ and ρ form a subalgebra of $\mathfrak{R}_3$; they must therefore be linearly dependent, and then $\mathfrak{A}_2$ is spanned by α_0 and ρ, and $r=0$. We may go one step further, and multiplying ρ by a suitable constant, replace it by α_1. For then it is always possible to find α_2 and α_3 to satisfy (35).

Second, $\mathfrak{R}_3$ is the only three-dimensional subalgebra of $\mathfrak{G}^{(0)}$. Indeed, if $\mathfrak{A}_3$ is such a subalgebra, then $\mathfrak{A}_3\bigcap\mathfrak{R}_3$ must be of dimension two or three. But two is impossible, as in the case of $\mathfrak{A}_2$, so $\mathfrak{A}_3$ and $\mathfrak{R}_3$ coincide.

We will classify the IW contractions of $\mathfrak{G}^{(0)}$ according to $\dim S_R$. Recall that once S_R is chosen, S_N, being irrelevant, can be chosen for convenience.

Case (a). $dim S_R=3$. Then (S_R forms a subalgebra) S_R is $\mathfrak{R}_3$. This contraction gives nothing new: $\mathfrak{G}^{(0)}$ and the contracted algebra are the same.

Case (b). $dim S_R=2$. Let S_R be spanned by α_0, α_1, and S_N by α_2, α_3. Then (nonsingular transformations in S_R contribute nothing significant) write

$$u\alpha_0=\alpha_0,\quad u\alpha_1=\alpha_1,\quad u\alpha_2=u\alpha_3=0.$$

On using (18) we obtain

$$[\alpha_1,\alpha_2]^{(1)}=\alpha_3,\quad [\alpha_3,\alpha_1]^{(1)}=\alpha_2,\tag{38}$$

and all other brackets vanish.

Case (c). $dim S_R=1$.

1. S_R spanned by α_0 and S_N chosen as $\mathfrak{R}_3$. This gives the four-dimensional Abelian algebra.

2. S_R spanned by α_1, and S_N by α_0, α_2, α_3. On writing

$$u\alpha_1=\alpha_1,\quad u\alpha_0=u\alpha_2=u\alpha_3=0,$$

we obtain, using (18),

$$[\alpha_1,\alpha_2]^{(1)}=\alpha_3,\quad [\alpha_3,\alpha_1]^{(1)}=\alpha_2,\tag{39}$$

and all other brackets vanish. This is seen to be the same as (38), or case (b).

3. S_R spanned by $\alpha_0+\alpha_1$, and S_N by $\alpha_0-\alpha_1$, α_2, α_3. On writing

$$u(\alpha_0+\alpha_1)=\alpha_0+\alpha_1,\quad u(\alpha_0-\alpha_1)=u\alpha_2=u\alpha_3=0,$$

and using (18), we obtain

$$[\alpha_0+\alpha_1,\alpha_2]^{(1)}=\alpha_3,\quad [\alpha_3,\alpha_0+\alpha_1]^{(1)}=\alpha_2,\tag{40}$$

and all other brackets vanish. This is again isomorphic to (38).

Case (d). $S_R=0$. This is the trivial contraction and gives the same result as case (c)1.

Thus IW contraction of $\mathfrak{G}^{(0)}$ gives algebras whose derived algebras are of dimension zero [cases (c)1; (d)], two [cases (b); (c)2,3], and three [case (a)]. In the latter case the contracted algebra is $\mathfrak{G}^{(0)}$ itself. The derived algebra of $\mathfrak{G}^{(1)}$ given by (37) is of dimension three, but $\mathfrak{G}^{(1)}$ is not isomorphic to $\mathfrak{G}^{(0)}$. To see this it is sufficient to note that the center of $\mathfrak{G}^{(1)}$ is in the derived algebra, which is not the case for $\mathfrak{G}^{(0)}$.

Furthermore, $\mathfrak{G}^{(1)}$ cannot be obtained from contraction, IW or general, of any of our other algebras with lower-dimensional derived algebras [cases (b)–(d)]. In fact contraction never increases the dimension of the derived algebra. This follows from quite general considerations. Assume the derived algebra of $\mathfrak{G}^{(0)}$ to be of dimension l, that of $\mathfrak{G}^{(1)}$ of dimension k. Let $\alpha_1,\cdots,\alpha_n$ span $\mathfrak{G}^{(0)}$, and consider the brackets $[\alpha_i,\alpha_j]$. These span the derived algebra of $\mathfrak{G}^{(0)}$. As $\lambda\to 0$, the brackets $[\alpha_i,\alpha_j]'=U(\lambda)^{-1}[U(\lambda)\alpha_i,U(\lambda)\alpha_j]$ converge to the $[\alpha_i,\alpha_j]^{(1)}$ and these span the derived algebra of $\mathfrak{G}^{(1)}$. Now given a set of vectors $\zeta_i(\lambda)$ converging to some limit set of linearly independent vectors $\zeta_i(0)$, it is clear in general that for small enough λ the $\zeta_i(\lambda)$ are also linearly independent. Thus if we choose from among the $[\alpha_i,\alpha_j]^{(1)}$ a set of k linearly independent ones, the corresponding $[\alpha_i,\alpha_j]'$ are also linearly independent for small enough λ. But so long as $\lambda\neq 0$, the algebra remains isomorphic to $\mathfrak{G}^{(0)}$, and therefore there are at

least k linearly independent vectors in its derived algebra. Thus $l \geq k$.

In conclusion, we see that (37) defines an algebra that cannot be obtained from $\mathfrak{G}^{(0)}$ by any number of IW contractions.

6. *Discussion*

The properties of the $\mathfrak{G}^{(i)}$ deduced in the foregoing do not exhaust the information contained in Eqs. (17) and (18). That this is so is evident from the fact that we have so far been unable to state in a simple group-theoretical way the content of these equations. It would be nice, for instance, to have a statement of the necessary and sufficient condition for contraction as simple as that given by IW (e.g., something like: a necessary and sufficient condition that $\mathfrak{G}^{(0)}$ be contracted by u is that the u^iS form subalgebras of $\mathfrak{G}^{(0)}$ for all i). No such statement equivalent to (17) has, however, been found.

Some insight into the difficulty involved is seen when one writes (17) in the form

$$[u\xi,u\eta]_N = u[\xi,u\eta]_N + u[u\xi,\eta]_N - u^2[\xi,\eta]_N. \quad (41)$$

This is a relation between the bracket of the mapping and the mapping of the bracket, but unlike for instance Eq. (19), it is quadratic in u. To obtain from it a general statement about the nature of $\mathfrak{G}^{(0)}$ and u would seem to be quite difficult.

All the foregoing analysis has been performed in the Lie algebras rather than in the groups. Since we have obtained the Lie algebra of the contracted group, we can find the corresponding universal covering group. We do not, however, know to which of the covered groups $G^{(0)}$ has contracted. If we were to study the way the topology of $G^{(0)}$ changes in the contraction (assuming it is known), we could find the topology of $G^{(1)}$ and hence which of the covered groups it is.

No topological analysis has been undertaken, but some qualitative remarks can be made. We recall that we start by considering a vector x in $G^{(0)}$ and then turn our attention to $\bar{x}$, which is given approximately by $x = U(\lambda)\bar{x}$, or $\bar{x} = U^{-1}(\lambda)x$ (say for x so close to the unit element that we may neglect quadratic and higher terms in its components). Now consider a small "volume" near the unit element of $G^{(0)}$. Under $U^{-1}(\lambda)$ this volume gets mapped into another, and the vectors defining this new volume are linear in $1/\lambda$. Thus as $\lambda \to 0$, the new volume increases without bound. In other words, from the topological point of view we may think of the process as an expansion. The topology itself remains unaltered until $\lambda = 0$, when it may change.

Consider, for instance, IW contraction of a group whose topology is that of a sphere. If S_1 in the Lie algebra is one-dimensional (corresponding to a one-parameter subgroup of $G^{(0)}$), the sphere is "stretched" into an ellipsoid, the topology remaining unaltered until $\lambda = 0$. In the limit, however, the major axis becomes infinite and the ellipsoid becomes a cylinder. Similarly, a group with cylindrical topology can be contracted into one with the topology of a plane. Thus we see that the connectivity of the contracted group may be either higher or lower than that of the original group. It seems equally clear that the contracted group is never compact. These topological remarks are of only qualitative nature and should not be taken too seriously.

A more complete discussion of topology for a particular example will be found in D. In D also one will find an analysis of the meaning of the successive contractions on the group, rather than on its Lie algebra.

II

A. Concerning Finite-Dimensional Representations

1. *Saving a Representation*

We shall deal in this section with representations of Lie algebras. By an m-dimensional representation of a Lie algebra we shall mean a mapping D of the elements ξ of a Lie algebra $\mathfrak{G}$ onto m-dimensional matrices X such that

$$D([\xi,\eta]) = D(\xi)D(\eta) - D(\eta)D(\xi) \equiv [D(\xi),D(\eta)]. \quad (42)$$

It is well known that a linear finite-dimensional representation of a Lie group induces such a representation of the group's Lie algebra. In this discussion we shall treat only finite-dimensional representations.

A mapping U of $\mathfrak{G}$ into itself induces a mapping W of D into itself according to

$$D'(\xi) = WD(\xi) = D(U\xi). \quad (43)$$

Because D is linear, the matrix of W is the same as that of U. In other words if $\alpha_1, \cdots, \alpha_n$ form a basis in $\mathfrak{G}$, and if $D(\alpha_i) = I_i$, then

$$I_i' = WI_i = D(U\alpha_i) = D(U_i{}^j\alpha_j) = U_i{}^jI_i. \quad (44)$$

Thus we may write U for W.

Our concern will, as before, be with λ-dependent U's, becoming singular when $\lambda = 0$, of the form

$$U(\lambda) = \lambda\mathbf{I} + (1-\lambda)u. \quad (45)$$

Then if $\xi \epsilon S_1$ and $D(\xi) = X$, we have

$$UX = \lambda X.$$

Thus when we go to the limit $\lambda = 0$ we find that $\mathfrak{G}_1^{(1)}$ is represented by the null matrix. The representation obtained in this way is therefore never faithful. (A faithful representation is one in which $D(\xi) = 0$ if and only if $\xi = 0$.)

This difficulty has already been pointed out by IW, who suggest two ways out of it, both involving varying

the representation in a λ-dependent way. The first is to consider a sequence of representations which converges to a representation of the contracted algebra. We shall not discuss this method here, although it is a very fruitful one. Since, in fact, the contracted group is never compact, this method must be used if the original representation of $\mathfrak{G}^{(0)}$ is finite-dimensional and one wants to obtain a unitary representation of $\mathfrak{G}^{(1)}$.

The second way out of the difficulty is to perform a λ-dependent similarity transformation on D. The representation so obtained remains, of course, equivalent to D so long as $\lambda \neq 0$. In the limit it becomes a representation of $\mathfrak{G}^{(1)}$. The object of the similarity transformation being to keep the representation of S_1 from vanishing in the limit, let us try to find an m-dimensional matrix $L(\lambda)$ such that

$$\lim_{\lambda \to 0} L^{-1}UXL \neq 0 \tag{46}$$

for $X = D(\xi)$ and for all $\xi \epsilon S$.

The problem we are faced with, then, is the following. Under what conditions is it possible to find an L satisfying (46) for which the representation of $\mathfrak{G}^{(1)}$ obtained will be a faithful one, what is an L that will produce this result, and what representations of $\mathfrak{G}^{(1)}$ can be so obtained? We shall say, when such an L has been found, that the representation is *saved*. Before proceeding, it should be noted that we have not been successful in solving this problem completely. We have, however, succeeded in discovering some properties of representations of $\mathfrak{G}^{(1)}$ obtained by saving representations of $\mathfrak{G}^{(0)}$, and it is to these results that this section is devoted.

As was remarked previously, it is essentially S_1 that concerns us, so that the first problem is to find an L such that

$$\lim_{\lambda \to 0} \lambda L^{-1}XL \neq 0$$

for all $\xi \epsilon S_1$ [or, as we shall say, for $X \epsilon D(S_1)$].

2. *Saving a Matrix*

Let us first try to save a single constant matrix I (or a one-dimensional S_1). We write

$$J_0 = \lim_{\lambda \to 0} J_\lambda = \lim_{\lambda \to 0} \lambda L^{-1}IL \neq 0, \tag{47a}$$

and assume L of the form

$$L = \sum \lambda^{a_i} L_i,$$

where the L_i are λ-independent, and $i = 0, 1, \cdots, r$ (the a_i are rational numbers, and we may set $0 = a_0 < a_1 < \cdots < a_r$ without loss of generality). Let d be the lowest common denominator of the a_i, so that $b_i = da_i$ are integers. Then writing

$$\lambda' = \lambda^{1/d}$$

we have (dropping the prime)

$$L = \sum \lambda^{b_i} L_i;$$

L is then what is called a λ matrix.[10] Equation (47a) now becomes

$$J_0 = \lim_{\lambda \to 0} \lambda^d L^{-1}IL \neq 0, \tag{47b}$$

with L a λ matrix. We shall attempt to find an L that will save I in the sense of (47b) for some integer d.

Now it is known[10] that for any λ matrix L there exist λ matrices A and B with determinant one such that

$$ALB = M = \sum_\mu P_\mu(\lambda) E_\mu. \tag{48}$$

Here the P_μ are polynomials in λ, and the E_μ are a complete set of projections (i.e., $E_\mu E_\nu = 0$ for $\mu \neq \nu$, while $E_\mu^2 = E_\mu$ and $\sum_\mu E_\mu = \mathbf{1}$). It is clear that the restriction to determinant one is not necessary. In fact for our purposes it will be convenient if the lowest power of λ in each of the P_μ has coefficient one. This is always possible to accomplish, given A and B, for instance by replacing B by

$$\sum \frac{1}{c_\mu} E_\mu B,$$

where c_μ is the coefficient of the lowest power of μ in P_μ (and hence nonzero). For our purposes, then, we shall speak of A and B which exist and have inverses for $0 \leq \lambda \leq 1$, and for which $c_\mu = 1$ for every μ. Now let us assume that I is saved by L [in the sense of (47b)]. Then using (48) we see that AIA^{-1} is saved by MB^{-1}. Further, since B and B^{-1} exist when $\lambda = 0$, AIA^{-1} is saved also by M.

We may thus consider the following problem: to find $A(\lambda)$, which exists together with its inverse at $\lambda = 0$, such that AIA^{-1} is saved by some M in the canonical form of Eq. (48). Then all possible AMB constructed out of such $A(\lambda)$, M, and $B(\lambda)$ (such that $B(0)$ and $B^{-1}(0)$ exist) will reproduce all possible L's that save I. Further, we can increase the class of possible L's if we remove the restriction that A and B be λ matrices (i.e., let their elements be irrational or transcendental functions of λ).

On proceeding, then, write

$$A = A_0 + \lambda A_1 + \lambda^2 A_2 + \cdots$$

and

$$A^{-1} = A_0^{-1} + \lambda \alpha_1 + \lambda^2 \alpha_2 + \cdots$$

for small enough values of λ. The α_i are easily calculated from the A_i, using the condition that $AA^{-1} = \mathbf{1}$ be λ-independent.

Let us now write

$$\tilde{I} = AIA^{-1} = I_0 + \lambda I_1 + \lambda^2 I_2 + \cdots. \tag{49}$$

[10] H. W. Turnbull and A. C. Aitken, *An Introduction to the Theory of Canonical Matrices* (Blackie and Son, Limited, England, 1932).

The I_i are easily calculated in terms of the A_i (through the α_i) and I.

We can now put (47b) in the form

$$J_0=\lim_{\lambda\to 0}\lambda^d BM^{-1}AIA^{-1}MB^{-1}$$

$$=\lim_{\lambda\to 0}B(\lambda^d M^{-1}\tilde{I}M)B^{-1}$$

$$=B(0)\tilde{J}_0B^{-1}(0)\neq 0 \qquad (50)$$

where we have used the fact that $B(0)$ and $B^{-1}(0)$ exist, and have written

$$\tilde{J}_0=\lim_{\lambda\to 0}\lambda^d M^{-1}\tilde{I}M.$$

Now J_0 will be nonzero if and only if $\tilde{J}_0$ is nonzero. Consider, therefore, the requirement that

$$\tilde{J}=\lambda^d M^{-1}\tilde{I}M$$

have a nontrivial (nonzero) limit as λ tends to zero, with M in the canonical form of (48). Note first that

$$M^{-1}=\sum_\mu \frac{1}{P_\mu(\lambda)}E_\mu,$$

so that

$$\tilde{J}=\lambda^d\sum_{\mu,\nu}\frac{P_\nu(\lambda)}{P_\mu(\lambda)}E_\mu\tilde{I}E_\nu.$$

Since we shall be interested only in the limit, we need consider only the lowest power of λ in each of the P_μ. Let this power be l_μ. Then

$$\tilde{J}_0=\lim_{\lambda\to 0}\tilde{J}=\lim_{\lambda\to 0}\sum_{\mu,\nu}\lambda^{d+l_\nu-l_\mu}E_\mu\tilde{I}E_\nu. \qquad (51)$$

We now change the notation in the following way. First, if for some $\rho\neq\sigma$ we have $l_\rho=l_\sigma$, we write $E_\rho+E_\sigma=E_\rho'$. In this way, to each *value* of l_μ we have now only one projection operator. Equivalent to this would be to replace the canonical form of (48) by a form of the type

$$ALB=M=\sum_i\lambda^i E_i. \qquad (52)$$

In fact we proceed in just this spirit with the E_μ (dropping the primes on the newly defined E_μ'), and write[11]

$$E_i=\begin{cases}0 & \text{if } i\neq l_\mu \text{ for any } \mu\\ E_\mu & \text{if } i=l_\mu \text{ for some } \mu.\end{cases}$$

This is equivalent to allowing all positive integers in (52). Then (51) becomes

$$\tilde{J}_0=\lim_{\lambda\to 0}\sum_{i,j}\lambda^{d+i-j}E_j\tilde{I}E_i$$

$$=\lim_{\lambda\to 0}\sum_{i,j,k}\lambda^{d+i-j+k}E_jI_kE_i,$$

where we have made use of (49). Finally, this can be written

$$\tilde{J}_0=\lim_{\lambda\to 0}\sum_k\lambda^{d-k}\sum_{i,j}E_jI_iE_{j-i-k}$$

if we write $E_i=0$ for $i<0$.

If this is to have any limit at all as $\lambda\to 0$, the coefficients of the negative powers of λ must vanish:

$$\sum_{i,j}E_jI_iE_{j-i-k}=0 \quad \text{for} \quad k>d.$$

Multiplying on the left and right by appropriate E's we arrive at

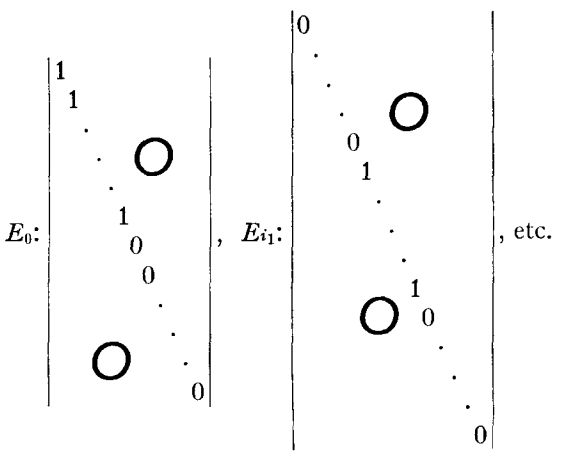
$$E_jI_iE_{j-i-k}=0 \quad \text{for} \quad k>d \quad \text{(NO SUM!)}. \qquad (53)$$

The limit (nonzero by assumption) is then

$$\tilde{J}_0=\sum_{i,j}E_jI_iE_{j-i-d}\neq 0. \qquad (54)$$

From this and (50) we get all the saved forms of I. Note that $B(0)$ is a quite arbitrary nonsingular matrix, so that we may think of it as inducing a coordinate transformation in the carrier space of the representation. It is then clearly irrelevant.

In order to discuss the meaning of (53) and (54), let us go to a coordinate system in which all of the E_i are diagonal. Then as is well known, they can be represented in the form



Here i_1 is the lowest nonzero value of i for which $E_i\neq 0$, and the first 1 in E_{i_1} appears on the main diagonal where the first 0 appears in E_0. In this coordinate system Eq. (54) signifies that $\tilde{J}_0$ will have nonzero elements only to the left of the main diagonal and that these elements will be those of the I_i. Exactly where to the left of the main diagonal they will occur depends on d and on the E_i. Equation (53) says that certain blocks to the left of the main diagonal must vanish in the I_i.

Recall that the problem was to find $A(\lambda)$. The problem is solved, to the extent that it is possible, by (53). Given d and M (or the E_i), the matrix $A(\lambda)$ must be such that the I_i calculated from it satisfy Eq. (53). There remains a great deal of arbitrariness

[11] Note that the form of L then implies that $E_0\neq 0$.

in this solution. First, d and the E_i can be quite freely chosen. Second, even when they are chosen, Eq. (53) does not specify $A(\lambda)$ at all uniquely.

One definite result of this discussion is that any matrix that is not a multiple of the unit matrix can be saved. (It is clear from the statement of the problem in (47b) that a multiple of the unit matrix cannot be saved.) For it is always possible to perform a (λ-independent) similarity transformation (we then write $A=A_0$) such that $I_0=A_0IA_0^{-1}$ has a nonzero element in the lower left-hand corner. Then let us choose d and the E_i so that d is the highest value of i for which $E_i\neq 0$ (recall that $E_0\neq 0$). With this choice, Eq. (53) is automatically satisfied, for then either E_j or E_{j-i-k} vanishes for $k>d$. As for (54), the only contribution comes when $i=0$ and $j=d$; this necessarily includes the element in the lower left-hand corner, and so $\tilde{J}_0\neq 0$.

3. *Saved Representation*

It is now evident that any single matrix can be saved if and only if it is not a multiple of the unit matrix. This does not mean that any representation can be save, even if $D(S_1)$ does not contain the unit element. In order that the representation be faithful, all of the basic vectors must be represented by linearly independent matrices. Since the saved matrices of $D(S_1)$ will have elements only to the left of the main diagonal, there cannot be more than $\frac{1}{2}m(m-1)$ of them if they are to be linearly independent. Thus if a representation is to be saved, it is necessary, though not sufficient, that

$$\dim S_1\leq\tfrac{1}{2}m(m-1).$$

The factor $\frac{1}{2}$ can be omitted if we allow complex representations of real algebras.

In this connection it may be desirable to maximize the number of nonzero elements of the saved matrices in an effort to keep them linearly independent. One might hope even to make all of the elements left of the main diagonal nonzero. Unfortunately this is not always possible. We demonstrate this for a single matrix I which we assume saved in the sense of (47a).

Let p be the degree of the minimal polynomial of I.[3] Then $(J_0)^p=0$. Indeed, consider

$$\begin{aligned}(\lambda L^{-1}IL)^p&=\lambda^pL^{-1}I^pL\\&=\lambda a_{p-1}\lambda^{p-1}L^{-1}I^{p-1}L+\lambda^2a_{p-2}\lambda^{p-2}L^{-1}I^{p-2}L\\&\qquad+\cdots+\lambda^pa_0,\end{aligned}$$

where the a_i are the negatives of the coefficients in the minimal polynomial

$$I^p-a_{p-1}I^{p-1}-\cdots-a_1I-a_0=0.$$

We then have

$$\begin{aligned}(\lambda L^{-1}IL)^p&=\lambda a_{p-1}(\lambda L^{-1}IL)^{p-1}\\&\qquad+\lambda^2a_{p-2}(\lambda L^{-1}IL)^{p-2}+\cdots+\lambda^pa_0.\end{aligned}$$

Because all the limits exist by assumption, we may allow λ to tend to zero, obtaining $(J_0)^p=0$. It then follows that

$$(\tilde{J}_0)^p=0.$$

Now $\tilde{J}_0$ has elements only to the left of the main diagonal. Let the elements on the diagonal just to the left of the main one be $j_1, j_2, j_3, \cdots, j_m$, and let e_i be the ith basis vector in the coordinate system in which J_0 has this form. Then a simple calculation shows that

$$(\tilde{J}_0)^le_i=j_ij_{i+1}j_{i+2}\cdots j_{i+l-1}e_{i+l}+f_{i+l+1},$$

where f_{i+l+1} involves only e_{i+l+1}, e_{i+l+2}, etc. (here we write $j_i=0$ if $i>m$, and similarly for e_i). Since $(J_0)^p=0$, there can be no more than $p-1$ nonzero j_i in a row. Thus unless the minimal polynomial of I is of degree m some of the elements on this diagonal of $\tilde{J}_0$ must vanish.

The principal and final result of interest for the saved representation may be stated in the form of the following

Theorem. Let Δ be the representation of $\mathfrak{G}^{(1)}$ obtained by saving a representation of D of $\mathfrak{G}^{(0)}$. Then Δ is reducible (though not necessarily completely reducible). Further, in the irreducible components of Δ the ideal $\mathfrak{G}_1^{(1)}$ (i.e., S_1) is represented entirely by null matrices.

Proof. Let $D(\alpha_i)=I_i$, where the α_i form a basis in S (note that these I_i are then not the same as the I_i discussed previously), and assume that a given L saves all of the I_i. Then there exists an $A(\lambda)$ such that the $\tilde{I}_i=AI_iA^{-1}$ are all saved by the same canonical M. Indeed, if we write $ALB=M$, we see that MB^{-1} and therefore also M saves all the $\tilde{I}_i$. Now let the saved matrices be $\tilde{J}_i$; i.e.,

$$\lim_{\lambda\to 0}\lambda^dM^{-1}\tilde{I}_iM=\tilde{J}_i,$$

and let $B(0)\tilde{J}_iB^{-1}(0)=J_i$. From the preceding it then follows that all the $\tilde{J}_i$ spanning $\Delta(S_1)$ have nonzero elements only below the main diagonal. Thus for any J_i spanning $\Delta(S_1)$ there is a coordinate system in the carrier space in which the J_i all have nonzero elements only below the main diagonal.

Let V be the carrier space on which Δ and D operate. Because of the form of the matrices in $\Delta(S_1)$, we have

$$\begin{aligned}\Delta(S_1)V&=V_1\subset V\\\Delta(S_1)V_1&=V_2\subset V_1\\&\vdots\\\Delta(S_1)V_q&=0.\end{aligned}$$

[$\Delta(S_1)V_i$ is the space spanned by Xv, where $X\in\Delta(S_1)$ and $v\in V_i$.]

Consider $X\in\Delta(S_1)$ and $Y\in\Delta(S)$. Then because S_1 forms the ideal $\mathfrak{G}_1^{(1)}$ in $\mathfrak{G}^{(1)}$,

$$[X,Y]=Z\in\Delta(S_1),$$

and Z maps V into V_1. Now for any $v\epsilon V$ we have

$$Y(Xv)=X(Yv)-Zv. \tag{55}$$

Because X also maps V into V_1, the two terms on the right are in V_1, and hence so is their sum. Further, all vectors in V_1 can be written in the form Xv with $X\epsilon\Delta(S_1)$. We therefore conclude that

$$YV_1\subseteq V_1$$

for all $Y\epsilon\Delta(S)$.

We could stop here, for we have reduced Δ and thus proven the first assertion of the theorem. It is, however, interesting and relevant to the proof of the second assertion that each of the V_i is invariant under (reduces) Δ.

To show this we proceed by induction. Assume that $YV_i\subseteq V_i$ for all $Y\epsilon\Delta(S)$. We choose X and Y as before, and consider $v\epsilon V_i$. Then we again arrive at (55), except that now both terms on the right are in V_{i+1}. Again, all vectors in V_{i+1} can be written in the form Xv with $X\epsilon\Delta(S_1)$ and $v\epsilon V_i$, so that we arrive at

$$YV_{i+1}\subseteq V_{i+1}.$$

Thus in general we may write

$$\Delta(S)V_i\subseteq V_i,$$

where

$$V=V_0\supset V_1\supset V_2\supset\cdots\supset V_q\supset V_{q+1}=0.$$

This proves that the V_i reduce Δ.

The second assertion of the theorem can be proven (as the first could have been) by exhibiting the forms of the matrices in Δ. We shall proceed differently, however.

Let W_i be subspaces of V such that $W_i\oplus V_{i+1}=V_i$, and let P_i be projection operators defined by some decomposition of the form $V=W_i\oplus T_{i+1}$, where $T_{i+1}\supseteq V_{i+1}$ (i.e., $P_iV=W_i$, $P_i^2=P_i$, $P_iT_{i+1}=0$). Let v be a vector in V_i. We may write $v=v_i+v_{i+1}$, where $v_i=P_iv\epsilon W_i$, and $v_{i+1}\epsilon V_{i+1}$. Now consider (with $X\epsilon\Delta$)

$$P_iXv=P_iXv_i+P_iXv_{i+1}.$$

Since X maps V_{i+1} into itself, $P_iXv_{i+1}=0$. Thus

$$P_iXv=P_iXP_iv.$$

It then follows, since for any $v\epsilon V$ we have $YP_iv\epsilon V_i$ if $Y\epsilon\Delta$, that

$$\begin{aligned}(P_iXP_i)(P_iYP_i)&=(P_iXP_i)(YP_i)\\&=P_iXYP_i.\end{aligned}$$

Thus the $P_i\Delta P_i$ form representations of $\mathfrak{G}^{(1)}$; they are, indeed, reduced components of Δ. They contain therefore all the irreducible components of Δ. Now consider P_iXP_i for any $X\epsilon\Delta(S_1)$. Since for any v we know that $P_iv\epsilon W_i\subset V_i$, and since X maps V_i into V_{i+1}, we find that $XP_iv\epsilon V_{i+1}$. Then $P_iXP_iv=0$, which completes the proof.

We thus see that the only irreducible representations obtained by saving are not faithful representations of the algebra. S_1 is always represented entirely by null matrices.

It is known[12] that any representation of a solvable Lie algebra can be made triangular (i.e., to have nonvanishing elements only on and below the main diagonal). In our case $\Delta(S_1)$ is more than triangular, for all the elements on the main diagonal vanish. By saving D, therefore, we do not obtain all the representations of $\mathfrak{G}^{(1)}$.

B. Exponents in Contraction

1. Local Exponents

In quantum mechanics one usually deals not with ordinary representations, but with ray representations. A unitary ray representation is a representation up to a factor by unitary operators. If $D(x)$ and $D(y)$ are the representatives of x and y in $G^{(0)}$, then

$$D(x)D(y)=e^{i\gamma(x,y)}D(xy).$$

This concept was first treated by Wigner[13] and was subsequently discussed in detail by Bargmann.[14] We will make use of Bargmann's terminology and results, though not his notation.

A local exponent of a group $G^{(0)}$ is any real valued continuous function $\gamma(x,y)$ which is defined for all elements x, y of some neighborhood and which satisfies the relations

$$\begin{aligned}\gamma(e,e)&=0\\\gamma(x,y)+\gamma(xy,z)&=\gamma(y,z)+\gamma(x,yz)\end{aligned} \tag{56}$$

(here e is the unit element of $G^{(0)}$). A trivial, or zero-equivalent local exponent is one for which there exists a function $\chi(x)$ such that

$$\gamma(x,y)=\chi(x)+\chi(y)-\chi(xy).$$

The question to which we direct our attention is the following. It is known that all of the local exponents for the Lorentz group are trivial. This is not true, however, of the Galilei group. How is it, then, that an exponent which starts out trivial becomes nontrivial when one goes to the limit $\lambda=0$? It turns out that this problem has a quite simple solution.

Consider a function $\chi(x;\lambda)$ which depends not only on x, but on the mapping φ (through λ). Then for every $\lambda>0$

$$\gamma(x,y;\lambda)=\chi(x;\lambda)+\chi(y;\lambda)-\chi(xy;\lambda) \tag{57}$$

is a trivial local exponent, so long as by xy we now mean the λ-dependent product.[15] This is still a local

[12] See, for instance, E. B. Dynkin, Uspekhi Mat. Nauk **2**, 59 (1947).

[13] E. P. Wigner, Ann. Math. **40**, 149 (1939).

[14] V. Bargmann, Ann. Math. **59**, 1 (1954).

[15] If we treat the φ^i of (5) as giving a sequence of mappings rather than of coordinate transformations (as we do in the Lie algebra), the product becomes λ-dependent in accordance with Eq. (8). This is the sense in which we speak of "the mapping φ" and the "λ-dependent product."

exponent for $G^{(0)}$, of course, for so long as $\lambda>0$, the group given by xy remains isomorphic to $G^{(0)}$.

Now if $\lim\chi(x;\lambda)$ as $\lambda\to 0$ exists, Eq. (57) gives a trivial local exponent of $G^{(1)}$ in the limit, for the product xy has as a limit the product in $G^{(1)}$. But even if $\chi(x;\lambda)$ has no limit, $\gamma(x,y;\lambda)$ may. Let us write

$$\lim_{\lambda\to 0}\gamma(x,y;\lambda)=\gamma^{(1)}(x,y).$$

Then $\gamma^{(1)}(x,y)$ is a local exponent (in general nontrivial) of $G^{(1)}$. To show this, one proves that $\gamma^{(1)}(x,y)$ satisfies equations similar to (56), namely,

$$\gamma^{(1)}(e,e)=0$$
$$\gamma^{(1)}(x,y)+\gamma^{(1)}(xy,z)=\gamma^{(1)}(y,z)+\gamma^{(1)}(x,yz).$$

Here the product is the contracted one (the product in $G^{(1)}$). We will not attempt to prove this here, but shall rather pass to the Lie algebra. Considerations similar to those of the Appendix can be used then to pass from the Lie algebra to the group. Similarly, it will be more convenient to discuss in the algebra the question of when the exponent so obtained is trivial.

2. *Lie Algebra*

To every equivalence class of local exponents there corresponds an equivalence class of infinitesimal exponents in the Lie algebra.[14] An infinitesimal exponent is defined as a real valued antisymmetric bilinear form $\Gamma(\xi,\eta)$ defined on the Lie algebra, such that

$$d\Gamma(\xi,\eta,\zeta)\equiv\Gamma([\xi,\eta],\zeta)+\Gamma([\eta,\zeta],\xi)+\Gamma([\zeta,\xi],\eta)=0. \quad (58)$$

Such an infinitesimal exponent is called trivial if there exists a linear function $X(\xi)$ defined on the algebra such that

$$\Gamma(\xi,\eta)=X([\xi,\eta]).$$

Then trivial infinitesimal exponents correspond to trivial local exponents, and vice versa.

We now define a trivial infinitesimal exponent

$$\Gamma(\xi,\eta;\lambda)=X([\xi,\eta]';\lambda) \quad (59)$$

[see Eq. (12)], where for fixed $0<\lambda\leqslant 1$ the function $X(\xi;\lambda)$ is linear in ξ. Further, we assume that although $\lim X(\xi;\lambda)$ as $\lambda\to 0$ does not exist in general for all ξ,

$$\lim_{\lambda\to 0}\Gamma(\xi,\eta;\lambda)=\lim_{\lambda\to 0}X([\xi,\eta]';\lambda)=\Gamma^{(1)}(\xi,\eta)$$

does exist for all ξ,η. Then $\Gamma^{(1)}$ is an infinitesimal exponent on $\mathfrak{G}^{(1)}$.

Indeed, it is clear that $\Gamma^{(1)}$ is linear and antisymmetric. All that remains is to show that it satisfies an equation similar to (58), namely,

$$d\Gamma^{(1)}(\xi,\eta,\zeta)=\Gamma^{(1)}([\xi,\eta]^{(1)},\zeta)+\Gamma^{(1)}([\eta,\zeta]^{(1)},\xi)+\Gamma^{(1)}([\zeta,\xi]^{(1)},\eta)=0. \quad (60)$$

We proceed as follows. Consider

$$\lim X([[\xi,\eta]',\zeta]';\lambda).$$

Since by assumption $\lim[\xi,\eta]'$ exists, we may write

$$[\xi,\eta]'=\rho+\sigma(\lambda),$$

where

$$\rho=[\xi,\eta]^{(1)},$$
$$\sigma(\lambda)=\sum\sigma^i(\lambda)\alpha_i\equiv\sigma^i\alpha_i.$$

Here the α_i, as usual, are basis vectors in S. The $\sigma^i(\lambda)$ are functions of λ (and of ξ and η) that vanish for all ξ and η when $\lambda=0$; i.e., $\sigma^i(0)=0$.

Since X is linear, we may thus write

$$\begin{aligned}\lim X([[\xi,\eta]',\zeta]';\lambda)&=\lim X([\rho+\sigma(\lambda),\zeta]';\lambda)\\&=\lim X([\rho,\zeta]'+[\sigma(\lambda),\zeta]';\lambda)\\&=\lim\{X([\rho,\zeta]';\lambda)+\sigma^i X([\alpha_i,\zeta]';\lambda)\}.\end{aligned}$$

As all limits exist and $\sigma^i(0)=0$, we finally have

$$\lim X([[\xi,\eta]',\zeta]';\lambda)=\lim X([[\xi,\eta]^{(1)},\zeta]';\lambda).$$

We now return to (60). We have

$$\begin{aligned}d\Gamma^{(1)}(\xi,\eta,\zeta)&=\lim X([[\xi,\eta]^{(1)},\zeta]';\lambda)+\text{cyclic perm.}\\&=\lim X([[\xi,\eta]',\zeta]';\lambda)+\text{cyclic perm.}\\&=\lim d\Gamma(\xi,\eta,\zeta;\lambda)\\&=0.\end{aligned}$$

Thus $\Gamma^{(1)}$ is an infinitesimal exponent on $\mathfrak{G}^{(1)}$.

$\Gamma^{(1)}$ is trivial if and only if there exists a linear function $X^{(1)}(\xi)$ such that $X^{(1)}([\xi,\eta]^{(1)})=\Gamma^{(1)}(\xi,\eta)$ for all $\xi,\eta\epsilon S$. Since $X^{(1)}$ is linear we may write

$$X^{(1)}(\xi)=\kappa_i\xi^i,$$

where the κ_i are constants. Then

$$\Gamma^{(1)}(\xi,\eta)=\kappa_i c_{jk}{}^i(0)\xi^j\eta^k,$$

where the $c_{jk}{}^i(0)$ are the contracted structure constants (the structure constants of $\mathfrak{G}^{(1)}$). On the other hand, we know that

$$X([\xi,\eta]';\lambda)=\theta_i(\lambda)c_{jk}{}^i(\lambda)\xi^j\eta^k$$

converges to $\Gamma^{(1)}(\xi,\eta)$ for all ξ,η. Thus $\Gamma^{(1)}$ is trivial if and only if there exist constants κ_i such that

$$\lim_{\lambda\to 0}\{\theta_i(\lambda)c_{jk}{}^i(\lambda)\}=\kappa_i c_{jk}{}^i(0). \quad (61)$$

It should be pointed out that although the $c_{jk}{}^i(\lambda)$ converge to the $c_{jk}{}^i(0)$ by assumption, we also assumed [see (59)] that the $\theta_i(\lambda)$ themselves do not converge. If they do, (61) is automatically satisfied with $\kappa_i=\theta_i(0)$.

3. *Inhomogeneous Two-Dimensional Lorentz Group*

As an example we shall show how such exponents, both trivial and nontrivial, may arise in the usual IW

contraction of the inhomogeneous two-dimensional Lorentz group to the corresponding Galilei group (this is the contraction performed in the introduction). Later we will see what relation this has to physical requirements.

The contraction is represented by going from Eq. (2) with $\lambda=1$ to Eq. (3) by passing to the limit in the reparametrization (4). Specifically, we write

$$x=\langle v,y,\tau\rangle.$$

and then the λ-dependent multiplication law is

$$x_2x_1=\langle v_2,y_2,\tau_2\rangle\langle v_1,y_1,\tau_1\rangle$$
$$=\left\langle \frac{v_1+v_2}{1+\lambda^2v_1v_2},\ y_2+g_2(\lambda)(y_1+v_2\tau_1),\right.$$
$$\left.\tau_2+g_2(\lambda)(\tau_1+v_2y_1\lambda^2)\right\rangle. \quad (62)$$

We have seemingly repeated Eq. (4) of the introduction to emphasize that when we think of the contraction in terms of a mapping, we focus our attention on fixed elements (say x_1 and x_2) of the group, and allow the multiplication law to vary in a λ-dependent way.

Now consider the function

$$\chi(x;\lambda)=(mc^2/\hbar)\tau=(m/\hbar\lambda^2)\tau \quad (63a)$$

defined on the group. On inserting this into (57) and using (62), we obtain the trivial exponent

$$\gamma(x_2,x_1;\lambda)=-(m/\hbar)\{\lambda^{-2}[g_2(\lambda)-1]\tau_1+g_2(\lambda)v_2y_1\}.$$

In the limit as $\lambda\to 0$, we have

$$\lim\gamma(x_2,x_1;\lambda)$$
$$=\gamma^{(1)}(x_2,x_1)=-(m/\hbar)\{\tfrac{1}{2}v_2^2\tau_1+v_2y_1\}. \quad (63b)$$

This is a local exponent on the Galilei group, and it can be shown to be nontrivial.[14] Note, by the way, that $\chi(x;\lambda)$ is not defined in the limit as λ tends to zero, yet the exponent it defines, as in the general discussion, tends to a limit.

A similar procedure, also with a χ that does not converge, may lead to a trivial exponent. Consider, for instance, the function

$$\chi(x;\lambda)=-v\lambda^{-2}.$$

A simple calculation will show that then

$$\gamma(x_2,x_1;\lambda)=\frac{1}{\lambda^2}\left(-v_1-v_2+\frac{v_1+v_2}{1+\lambda^2v_1v_2}\right)$$

which converges to

$$\gamma^{(1)}(x_2x_1)=-(v_1+v_2)v_1v_2.$$

This $\gamma^{(1)}$ can be obtained, however, from the function

$$X^{(1)}(x)=v^3/3,$$

by the usual formula [the analog of (57)], and thus is trivial.

Without going into detail we shall repeat this in the Lie algebra. For the two-dimensional Lorentz group we have

$$[\alpha_1,\alpha_2]=\alpha_3,\quad [\alpha_2,\alpha_3]=0,\quad [\alpha_3,\alpha_1]=-\alpha_2$$

(α_1 generates the pure Lorentz transformations, α_2 the space translations, and α_3 the time translations). The contraction is obtained by the mapping

$$U(\lambda)\alpha_1=\lambda\alpha_1,\quad U(\lambda)\alpha_2=\lambda\alpha_2,\quad U(\lambda)\alpha_3=\alpha_3,$$

so that

$$[\alpha_1,\alpha_2]'=\lambda^2\alpha_3,\quad [\alpha_2,\alpha_3]'=0,\quad [\alpha_3,\alpha_1]'=-\alpha_2,$$

and

$$[\alpha_1,\alpha_2]^{(1)}=0,\quad [\alpha_2,\alpha_3]^{(1)}=0,\quad [\alpha_3,\alpha_1]^{(1)}=-\alpha_2. \quad (64)$$

We now define

$$X(\xi;\lambda)=(m/\hbar\lambda^2)\xi^3,$$

where ξ^3 is the third component of ξ (λ^2 is, of course, the square of λ). Inserting this into (59) we have

$$\Gamma(\xi,\eta;\lambda)=-(m/\hbar)(\xi^2\eta^1-\xi^1\eta^2).$$

Since this is λ-independent, $\Gamma^{(1)}=\Gamma$; for $\mathfrak{G}^{(0)}$ this is a trivial infinitesimal exponent, for $\mathfrak{G}^{(1)}$ a nontrivial one.

The nontriviality can be seen very simply in this case. Let us check it, however, using (61). With our choice of $X(\xi;\lambda)=\theta_i(\lambda)\xi^i$ we have

$$\theta_1=0,\quad \theta_2=0,\quad \theta_3=m/\hbar\lambda^2.$$

The λ-dependent structure constants are

$$c_{12}{}^2(\lambda)=-c_{21}{}^3(\lambda)=\lambda^2,\quad c_{31}{}^2(\lambda)=-c_{13}{}^2(\lambda)=-1,$$

and all others vanish. The contracted structure constants are

$$c_{31}{}^2(0)=-c_{13}{}^2(0)=-1,$$

and all others vanish. Thus the only nonzero expressions of the form $\theta_ic_{jk}{}^i$ are

$$\theta_ic_{jk}{}^i=\theta_3c_{12}{}^3=-\theta_3c_{21}{}^3=m/\hbar,$$

while for any set of κ_i, the only nonvanishing $\kappa_ic_{jk}{}^i(0)$ is

$$\kappa_2=\kappa_ic_{31}{}^i.$$

Thus (61) cannot be satisfied, and $\Gamma^{(1)}$ is therefore nontrivial.

On the other hand, the choice $X(\xi;\lambda)=-\xi^1/\lambda^2$ (which corresponds to $\chi=-v/\lambda^2$) leads to $\Gamma^{(1)}=\Gamma=0$, which is, of course, trivial. A nonvanishing trivial $\Gamma^{(1)}$ can be obtained, for instance, from $X=\xi^3/\lambda+\xi^2$. This gives

$$\Gamma^{(1)}=\xi^1\eta^3-\xi^3\eta^1,$$

which can be obtained from

$$X^{(1)}(\xi)=\kappa_1\xi^1+\kappa_2\xi^2$$

with arbitrary κ_1, κ_2.

The exponent of (63b) arises when one deals with the transformation properties of a function satisfying the Schrödinger equation.[14,16] It may be deduced from the requirement that the Schrödinger equation be invariant under Galilei transformations. We might, however, also proceed differently.

Starting with a wave function which is a solution of a relativistic equation (we will take the Klein-Gordon equation) we may pass in the usual way to the nonrelativistic limit. By studying how the relativistic wave function transforms we can deduce a transformation law in the limit for the nonrelativistic function. It will be found that a trivial exponent must be introduced if this transformation law is to converge. This exponent is not uniquely determined, but if chosen in agreement with (63a) the divergence is eliminated. It leads, of course, to the nontrivial exponent of (63b).

Let us consider a positive-energy solution of the free-particle Klein-Gordon equation. We write (up to a normalizing constant)

$$\Psi(x)=\int\Phi(p)e^{ip\cdot x/\hbar}dV$$

where $x=(\mathbf{x},ct)$ and $p=\{\mathbf{p},+(m^2c^2+\mathbf{p}^2)^{\frac{1}{2}}\}$ are the position and momentum four-vectors, and dV is an invariant volume element. We shall not be concerned with questions of convergence; let us assume, therefore, that Φ drops off sufficiently rapidly at infinity to provide convergence of the integral. As we shall be interested in the nonrelativistic limit and are not concerned with normalization, we choose a volume element which has a limit as $1/c$ approaches zero:

$$dV=mc(d^3p/p^0)=d^3p/(1+\mathbf{p}^2/m^2c^2)^{\frac{1}{2}}.$$

We have written $p\cdot x=cp^0t-\mathbf{p}\cdot\mathbf{x}$. In the preceding expression for Ψ all of the c dependence is exhibited, except that Φ may depend on c through p^0. We shall assume that this c dependence is absent in a given coordinate system, and it then follows that in any other coordinate system related to the first by a homogeneous Lorentz transformation the c dependence is such that Φ has a limit as $1/c$ tends to zero (see the following).

Since $\Psi(x)$ is a scalar function, we know that under a Lorentz transformation Λ it transforms according to

$$\Psi'(x)=\Psi(\Lambda^{-1}x).$$

A simple calculation using the invariance of dV and $p\cdot x$ under Lorentz transformations then shows that the momentum-space wave function transforms according to

$$\Phi'(p)=\Phi(L^{-1}p) \tag{65a}$$

if $\Lambda=L$ is a homogeneous Lorentz transformation. If we assume Φ to depend only on $\mathbf{p}$ (not on p^0) and hence to be c independent, we see that Φ' depends on c. But this dependence is through the space components of $L^{-1}p$, and these have limits as $1/c\to 0$. Thus Φ has a limit as $1/c$ tends to zero.

A similar calculation shows that

$$\Phi'(p)=\Phi(p)e^{ip\cdot y/\hbar} \tag{65b}$$

if Λ is a translation by the four-vector $y=(\mathbf{y},c\tau)$.

Now let us consider the Fourier expansion of Ψ in more detail. We have

$$\begin{aligned}\Psi(x)&=\int dV\Phi(p)e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\exp[-imc^2t(1+\mathbf{p}^2/m^2c^2)^{\frac{1}{2}}/\hbar]\\&=\int dV\Phi(p)e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\\&\quad\times\exp[-imc^2t(1+\mathbf{p}^2/2m^2c^2+\cdots)/\hbar]\\&=e^{-iEt/\hbar}\int dV\Phi(p)e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\\&\qquad\times\exp\{-i[\mathbf{p}^2t/2m\hbar+O(1/c^2)]\},\end{aligned}$$

where $E=mc^2$ goes as c^2. Thus $\Psi(x)$ has no limit as $1/c\to 0$, but $\Psi(x)e^{iEt/\hbar}$ has a limit. We then define the nonrelativistic wave function as

$$\begin{aligned}\psi(\mathbf{x},t)&=\lim_{c\to\infty}\Psi(x)e^{iEt/\hbar}\\&=\int d^3p[\lim_{c\to\infty}\Phi(p)]\exp[i(\mathbf{p}\cdot\mathbf{x}-\mathbf{p}^2t/2m)/\hbar].\end{aligned}$$

The multiplication by $e^{-iEt/\hbar}$ corresponds just to subtracting out the rest energy from the wave function, or calculating the energy, as one ordinarily does in nonrelativistic mechanics, with respect to this rest energy.

We now compare this expression with the relation (again disregarding normalization)

$$\psi(\mathbf{x},t)=\int d^3p\phi(\mathbf{p})\exp[i(\mathbf{p}\cdot\mathbf{x}-\mathbf{p}^2t/2m)/\hbar]$$

for the nonrelativistic free particle. Then the nonrelativistic momentum-space wave function can be seen to be given in terms of the relativistic one by

$$\phi(\mathbf{p})=\lim_{c\to\infty}\Phi(p).$$

We now define the transformed nonrelativistic function by

$$\phi'(\mathbf{p})=\lim_{c\to\infty}\Phi'(p).$$

This leads to the following transformation laws for ϕ.

[16] W. Pauli, *Handbuch der Physik* (Springer-Verlag, Berlin, 1933), Vol. XXIV, p. 1.

(a) A pure rotation R:

$$\phi_R(\mathbf{p})=\phi(R^{-1}\mathbf{p}).$$

(b) A pure Lorentz transformation to a frame moving with velocity $\mathbf{v}$:

$$\phi_v(\mathbf{p})=\phi(\mathbf{p}-m\mathbf{v}).$$

(c) A space translation by an amount $\mathbf{y}$:

$$\phi_y(\mathbf{p})=\phi(\mathbf{p})\exp(-i\mathbf{p}\cdot\mathbf{y}/\hbar).$$

(d) A time translation by an amount τ:

$$\phi_\tau(\mathbf{p})=\lim_{c\to\infty}\Phi(p)\exp(ip^0c\tau/\hbar).$$

This last expression has no limit. We can overcome this difficulty by introducing an exponent into (65b). Since this will introduce just a phase factor, it involves no physical change.

We may write

$$\begin{aligned}\Phi(p)\exp(ip^0c\tau/\hbar)&\\ =\Phi(p)\exp[imc^2\tau(1+\mathbf{p}^2/2m^2c^2+\cdots)/\hbar]&\\ =e^{iE\tau/\hbar}\Phi(p)\exp\{i[\mathbf{p}^2\tau/2m\hbar+O(1/c^2)]\}.&\end{aligned}$$

It is seen that a natural choice for the exponent is that of (63a), for this involves just multiplying by $e^{-iE\tau/\hbar}$ and thus eliminating the factor that fails to converge. We thus replace (65a) and (65b), respectively, by

$$\Phi'(p)=\omega(\Lambda)\Phi(L^{-1}p),$$
$$\Phi'(p)=\omega(\Lambda)\Phi(p)e^{ip\cdot y/\hbar},$$

where

$$\omega(\Lambda)=e^{-iE\tau/\hbar},$$

and τ is the time translation in Λ. Note that it is just this kind of p-independent factor we would like to introduce into the transformation law for the wave function. With it our results (a), (b), and (c) remain the same, and (d) becomes

$$\phi_\tau(\mathbf{p})=\phi(\mathbf{p})\exp(i\mathbf{p}^2/2m\hbar).$$

As was mentioned, this gives the correct transformation law for the Schrödinger-equation wave function [i.e., (63a) leads to the nontrivial exponent of (63b)]. We have obtained it here from the requirement that the relativistic wave function transform in a way that has a nonrelativistic limit.

4. *Concluding Remarks*

With respect to representations, the major outstanding problem is that of infinite-dimensional representations, which is certainly of greater interest both from the physical and mathematical points of view. One question that may be asked, for instance, is whether or not all unitary representations of the contracted group can be obtained from those of the original group.

Another problem involving contraction, particularly interesting from the physical point of view, is to find all groups (or algebras) that contract to a given one. Work is being undertaken in both of these directions.

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APPENDIX

It can be shown that a limit for the multiplication law follows from a limit for the structure constants. A proof of this assertion is sketched in the following.[17]

Let

$$|\xi|=[\textstyle\sum_i|\xi^i|^2]^{\frac{1}{2}} \tag{A1}$$

define a norm in the Lie algebra for any ξ (the ξ^i are the coordinates of ξ in some coordinate system). It is then a simple matter to show that

$$|[\xi,\eta]|\leq\gamma|\xi||\eta|,$$

where

$$\gamma=[\textstyle\sum_{i,j,k}|c_{jk}{}^i|^2]^{\frac{1}{2}}.$$

We may define a norm in the Lie group in the same way, using canonical coordinates. That is, if ξ is mapped by the exponential mapping[18] onto the group element $\exp\xi=x$, the canonical coordinates of x are the ξ^i. Henceforth, then, in this Appendix we will use the same symbol ξ for the element of the algebra and the group element x. Then the norm of the group element ξ is again given by (A1).

We shall prove the original assertion in terms of this norm in canonical coordinates.

Now in canonical coordinates the group product can be expressed by the Baker-Hausdorff series. This means that if ξ and η are elements of the group, their product $\zeta=\xi\eta$ can be written in the form

$$\zeta=\sum_{l=0}^{\infty}\zeta_l, \tag{A2}$$

where the ζ_l are given by the recursion relation

$$\begin{aligned}&\zeta_0=0,\\ &\zeta_1=\xi+\eta,\\ &(l+1)\zeta_{l+1}=\tfrac{1}{2}[\xi-\eta,\zeta_l]\\ &\qquad+\textstyle\sum\kappa_{2m}[\zeta_{\mu1}[\zeta_{\mu2}[\cdots[\zeta_{\mu2m},\xi+\eta]\cdots].\end{aligned} \tag{A3}$$

[17] The method of proof is due to Professor Bargmann.

[18] P. M. Cohn, *Lie Groups* (Cambridge University Press, New York, 1957).

Here the sum is taken over all positive integers m and μ_i such that $\mu_1+\mu_2+\cdots+\mu_{2m}=l$. The κ_{2m} are the coefficients in the power-series expansion

$$\frac{\zeta}{2}\coth\frac{\zeta}{2}=\sum_0^\infty \kappa_{2m}\zeta^{2m}$$

(they are related to the Bernoulli numbers). The bracket operation in (A3) is, of course, defined for the elements in the Lie algebra, but the results of the operations are then interpreted as elements in the Lie group with the given canonical coordinates. This defines the Baker-Hausdorff series.

It can be shown that with the norm of (A1) this series converges uniformly for $|\xi|+|\eta|\leq\pi/4\gamma^*$ (where $\gamma^*>\gamma$), or in a hypersphere of radius $\pi/(8\gamma^*)$. Very roughly, this may be proven in the following way. By using (A3) and the values of the κ_{2m}, one shows that

$$(l+1)|\zeta_{l+1}|\leq\Big(\sum_{n\leq\Sigma\mu_i=l} k_n\gamma^n|\zeta_{\mu_1}|\cdots|\zeta_{\mu_n}|\Big)\delta, \quad \text{(A4)}$$

where

$$k_n=4/(2\pi)^n, \quad \delta=|\xi|+|\eta|.$$

One then considers the power series

$$f(z)=\sum\alpha_l z^l, \quad \text{(A5)}$$

whose coefficients are defined by

$$\alpha_0=0$$

$$(l+1)\alpha_{l+1}=\Big(\sum_{n\leq\Sigma\mu_i=l} k_n\gamma^n\alpha_1\cdots\alpha_n\Big)\delta.$$

It is clear that $|\zeta_l|\leq\alpha_l$, so that convergence of the series

$$\zeta(z)=\sum\zeta_l z^l \quad \text{(A6)}$$

is implied by convergence of (A5). By noting that $df/dz=4\delta(1-\gamma f/2\pi)^{-1}$ and solving for f with the condition $f(0)=0$, one finds that

$$f=(2\pi/\gamma)[1-(1-4\gamma\delta z/\pi)^{\frac{1}{2}}] \quad \text{(A7)}$$

(take the positive root), which means that (A5) converges for $z\leq\pi/4\gamma\delta$. Since we are dealing with a power series, the convergence is uniform on any closed set entirely within the circle of convergence, or for $z\leq\pi/4\delta\gamma^*$, where $\gamma^*>\gamma$. If we set $z=1$, Eq. (A6) gives ζ, and we thus find that the Baker-Hausdorff series converges uniformly if

$$\delta=|\xi|+|\eta|\leq\pi/4\gamma^* \quad \text{(A8)}$$

(or in a hypersphere of radius $\pi/8\gamma^*$).

Now consider a sequence of structure constants converging to a limit, and hence a sequence of γ's with a limit. Let γ^* be greater than all the γ's of the sequence (or greater than all γ's past a certain one). Then for δ given by (A8) the Baker-Hausdorff series converges uniformly, and the multiplication law is thus a continuous function of the structure constants. It thus approaches a limit together with the structure constants, and this limit is obtained in the usual way from the limit values of the structure constants (e.g., by the Baker-Hausdorff series).

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Complex Orthogonal and Antiorthogonal Representation of Lorentz Group

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By using the fact that a plane electromagnetic wave is described by two Lorentz invariant statements, a complex orthogonal representation of the Lorentz group, including charged fields, is discussed. The representation provides the possibility of a combined study of the P, C, T symmetry operations for spin $\frac{1}{2}$ and spin 1 fields. In particular, the chargelessness of the neutrino as a complex fermion field results from a reducible three charge states representation of the complex group.

I. INTRODUCTION

IT is well known that to every relativistic quantum-mechanical system of equations corresponds a representation of Lorentz group. The knowledge of a certain representation of Lorentz group is a more general concept than a particular quantum-mechanical equation. It is, therefore, quite desirable to further discuss the known representations of Lorentz group. In this paper we consider some simple features of the three-dimensional complex representations.

Real orthogonal transformations in three-dimensional Euclidean space are homomorphic onto unitary transformations in the spinor plane. The proper Lorentz transformations as a six-parameter representation of homogeneous Lorentz group, together with improper Lorentz transformations, can be expected to have a complex orthogonal representation.

The three-dimensional unitary space, because of its Euclidean nature and also because of the requirement of eight parameters for the irreducible representation of the three-dimensional unitary unimodular group, cannot be used for the representation of homogeneous Lorentz group. For the representation of the Lorentz group we may envisage a three-dimensional linear manifold spanned by the special type of complex vectors formed from the space and time components of an antisymmetric tensor field.

A representation of the Lorentz group by a three-dimensional complex orthogonal group is also suggested from the fact that the Lorentz invariant path length $dp^2=0$ of a plane electromagnetic wave can be replaced by the two Lorentz invariant statements that the electric and magnetic vectors of the wave are (i) of equal magnitude and (ii) perpendicular to one another. At each point of the wave we can set up an "invariant coordinate system" with electric vector E and magnetic vector H by choosing the third axis of the coordinate system in the direction of its spin.

II. COMPLEX GROUP

Let $\phi_{\alpha\beta}$ be any four-dimensional antisymmetric tensor function of coordinates and time. We define a complex three-dimensional ket-vector $|\chi\rangle$ by

$$|\chi\rangle=\begin{pmatrix}\chi_1\\ \chi_2\\ \chi_3\end{pmatrix} \tag{II.1}$$

where

$$\chi_i=\phi_{4i}+\tfrac{1}{2}i\epsilon_{ijk}\phi_{jk},$$

and ϕ_{4i} and ϕ_{ij} are time and space parts of $\phi_{\alpha\beta}$. The Latin and Greek indices run from 1 to 3 and 1 to 4, respectively. The quantities ϵ_{ijk} are the usual three-dimensional Levi-Cevita symbols.

We shall use the symbol $(\chi|$ to mean just the transpose of the ket $|\chi\rangle$, while the symbol $\langle\chi|$ for the transpose and complex conjugation of the ket $|\chi\rangle$, viz.,

$$(\chi|=[\chi_1,\chi_2,\chi_3]$$
$$\langle\chi|=[\chi_1^*,\chi_2^*,\chi_3^*]=(|\chi\rangle)^\dagger.$$

We must distinguish between the two ways of squaring of a complex vector $|\chi\rangle$ belonging to the three-dimensional complex space:

(i) Lorentz invariant square of $|\chi\rangle$ is

$$(\chi|\chi)=\chi_1^2+\chi_2^2+\chi_3^2. \tag{II.2}$$

(ii) Hermitian (or gauge-invariant) square of $|\chi\rangle$ is

$$\langle\chi|\chi\rangle=|\chi_1|^2+|\chi_2|^2+|\chi_3|^2. \tag{II.3}$$

The expression (II.3) is invariant with respect to a gauge transformation

$$|\chi_\delta\rangle=e^{i\delta}|\chi\rangle, \tag{II.4}$$

where $\delta(x)$ is an arbitrary invariant function of space and time. All vectors of the complex three-dimensional manifold are of the form (II.4) or its complex conjugate.

The ket $|\chi_\delta\rangle$ can further be qualified as a complex vector by its transformation properties. For this purpose we introduce complex orthogonal transformations which leave Eq. (II.2) unchanged. If R is the transformation matrix of a complex ket, we obtain another ket belonging to the same complex space by

$$|\chi'\rangle=R|\chi_\delta\rangle=Re^{i\delta}|\chi\rangle. \tag{II.5}$$

Hence

$$(\chi'|\chi')=(\chi|e^{i\delta}R^\dagger Re^{i\delta}|\chi),$$

so that the invariance of Eq. (II.2) under R transformations requires that all R transformations must

satisfy the conditions

$$\tilde{R}R=R\tilde{R}=e^{-2i\delta}, \tag{II.6}$$

where $\tilde{R}$ is the transpose of R. These conditions on R correspond to six complex or 12 real equations so that of the 18 parameters (plus the phase δ) fixing R only six are independent. The six parameters together with a given $\delta(x)$ will fix a member of the complex group [or extended complex group for $\delta(x)\neq 0$].

We shall be interested in the two subgroups of the extended group corresponding to special values of gauge parameter $\delta(x)$.

(i) $\delta(x)=0$, $\delta(x)=\pi$, and

$$\tilde{R}R=R\tilde{R}=I_3. \tag{II.7}$$

This is the complex orthogonal group. The determinant of R is $+1$ or -1. Thus, as in the real group, one has to distinguish between pure complex rotation group with determinant $+1$ and rotation-reflection group which includes transformation matrices with determinant -1. The identity element of the group is the unit matrix I_3. Because of the nonunitary character of R, its eigenvalues are not all of unit magnitude.

(ii) $\delta(x)=\frac{1}{2}\pi$ and

$$\tilde{R}R=R\tilde{R}=-I_3. \tag{II.8}$$

This is the antiorthogonal group. The determinant of R (in cases where it exists) in this case is $+i$ or $-i$. We shall see that antiorthogonal R transformations are equivalent to antilinear operations[1] on the vectors of the complex space.

The complex conjugate of any ket $|\chi\rangle$ is transformed by the complex conjugates of R transformations satisfying the orthogonality and antiorthogonality conditions,

$$\tilde{R}^*R^*=R^*\tilde{R}^*=I_3, \tag{II.9}$$

and

$$\tilde{R}^*R^*=R^*\tilde{R}^*=-I_3, \tag{II.10}$$

respectively. If $\bar{C}$ is the operator of complex conjugation (antiunitary operator), then it can operate on $|\chi\rangle$ to yield

$$|\chi^*\rangle=\bar{C}|\chi\rangle$$

and

$$|\chi'^*\rangle=\bar{C}|\chi'\rangle=\bar{C}R|\chi\rangle=\bar{C}R\bar{C}|\chi^*\rangle=R^*|\chi^*\rangle,$$

where we used the antiunitary property[2]

$$\bar{C}^2=1. \tag{II.11}$$

For the proper complex orthogonal group a member R of the group can be connected to the unit element I_3 of the group by assuming that it is a continuous function of an arbitrary parameter τ. In this case, from differentiating Eq. (II.7), it can easily be shown that R satisfies the equation

$$idR/d\tau=ZR, \tag{II.12}$$

where Z is a complex antisymmetric 3×3 matrix, i.e.,

$$\tilde{Z}=-Z,$$

and

$$Z=i\begin{bmatrix} 0 & -a_3-ib_3 & a_2+ib_2 \\ a_3+ib_3 & 0 & -a_1-ib_1 \\ -a_2-ib_2 & a_1+ib_1 & 0 \end{bmatrix}$$

$$=\sum_{j=1}^{3}[a^jK_j+ib^jK_j], \tag{II.13}$$

where a^j and b^j $(j=1,2,3)$ are real numbers, and K_j are the spin matrices of the electromagnetic field and are given by

$$K_j=\begin{bmatrix} 0 & -i\delta_{j3} & i\delta_{j2} \\ i\delta_{j3} & 0 & -i\delta_{j1} \\ -i\delta_{j2} & i\delta_{j1} & 0 \end{bmatrix}. \tag{II.14}$$

The Hermitian matrices K_j together with the anti-Hermitian matrices iK_j are the generators of the complex infinitesimal rotations in complex space.

For τ-independent Z the typical R transformations are given by

$$\begin{aligned} R_1&=\exp[i(\psi+i\lambda)K_1] \\ R_2&=\exp[i(\phi+i\epsilon)K_2] \\ R_3&=\exp[i(\theta+i\rho)K_3]. \end{aligned} \tag{II.15}$$

A Lorentz transformation of the electromagnetic field can be affected by a complex orthogonal matrix. For example, the transformation by R_1 corresponds to a rotation around x_1 direction by an angle ψ and a uniform motion along the same direction with a velocity v, where

$$\tan\psi=v/c.$$

From

$$|\chi'>=R_1\chi|>, \tag{II.16}$$

we obtain

$$\begin{aligned} \chi_1'&=\chi_1 \\ \chi_2'&=\gamma\left[\chi_2\left(\cos\psi-i\frac{v}{c}\sin\psi\right)\right. \\ &\qquad \left.+\chi_3\left(\sin\psi+i\frac{v}{c}\cos\psi\right)\right] \\ \chi_3'&=\gamma\left[-\chi_2\left(\sin\psi+i\frac{v}{c}\cos\psi\right)\right. \\ &\qquad \left.+\chi_3\left(\cos\psi-i\frac{v}{c}\sin\psi\right)\right], \end{aligned} \tag{II.17}$$

[1] E. P. Wigner, *Group Theory* (Academic Press, Inc., New York, 1959), contains a detailed discussion of antilinear operations in physics. In connection with a discussion of vacuum expectation values of time-ordered products of field operators, D. Hall and A. S. Wightman have introduced a complex representation of Lorentz group [Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **31**, No. 5 (1957)]. Their discussion is, however, meant for quite a different purpose and is not directly related to the present work.

[2] The subgroup of the extended group considered here is a four branch group corresponding to four different values of the determinants of R transformations.

where

$$\gamma=(1-v^2/c^2)^{-\frac{1}{2}}.$$

For $\psi=0$, these are the usual Lorentz transformation formulas of the electromagnetic field.

III. CHARACTERISTIC MATRICES OF THE COMPLEX GROUP

As a simple example to illustrate the role of complex group we consider the complex ket $|\eta\rangle$ defined by

$$|\eta\rangle=\tilde{K}^\mu p_\mu|\chi\rangle, \tag{III.1}$$

where p_μ is the momentum four-vector of a particle and $\tilde{K}_\mu$ are the transpose of K_μ and where

$$K^4=K_4=I_3, \quad \tilde{K}_i=-K_i.$$

We shall use the Lorentz metric $a_{\mu\nu}$ defined by

$$a_{i4}=a_{4i}=0, \quad a_{44}=1, \quad a_{ij}=-\delta_{ij}$$

to raise and lower tensor indices. The symbol F corresponds to the matrix form of $a_{\mu\nu}$,

$$F=[a_{\mu\nu}]. \tag{III.2}$$

Now, the Lorentz invariance of Eq. (III.1) can be studied by forming the quantity

$$(\eta|\eta)=(\chi|K^\mu p_\mu\tilde{K}^\nu p_\nu|\chi),$$

where

$$K^\mu p_\mu\tilde{K}^\nu p_\nu=p_4{}^2-(\mathbf{K}\cdot\mathbf{p})^2,$$

and

$$(\mathbf{K}\cdot\mathbf{p})^2=p^2-\mathbf{pp}.$$

Hence

$$(\eta|\eta)=(\chi|p_\mu p^\mu|\chi)+(\mathbf{p}\cdot\boldsymbol{\chi})^2,$$

which with the condition

$$\mathbf{p}\cdot\boldsymbol{\chi}=p_1\chi_1+p_2\chi_2+p_3\chi_3=0, \tag{III.3}$$

becomes a Lorentz invariant expression. In particular, if $|\eta\rangle=0$ and $p_\mu=-i\hbar\partial/\partial x^\mu$, then Eqs. (III.1) and (III.3) are Maxwell's equations for charge free electromagnetic[3] field,

$$\begin{aligned} &i\hbar(\partial/\partial t)|\chi\rangle=H|\chi\rangle, \\ &\boldsymbol{\nabla}\cdot\boldsymbol{\chi}=0, \end{aligned} \tag{III.4}$$

where

$$H=c\mathbf{K}\cdot\mathbf{p}. \tag{III.5}$$

For the kets $|\chi\rangle$ satisfying Maxwell's equations (III.4) and (III.5) the corresponding space is a special representation of the more general complex space. In this case K_μ matrices (to be shown later) transform like a four-vector. The most general discussion of the complex space, without the restriction of chargelessness of the field, can be based on the transformation properties of energy and momentum of the electromagnetic field in the complex representation.

We first note that any symmetric tensor $T_{\mu\nu}$ of the Maxwellian form

$$T_{\mu\nu}=\tfrac{1}{2}\Omega a_{\mu\nu}-\phi_\mu\phi_\nu{}^\rho, \tag{III.6}$$

satisfies

$$\begin{aligned} T_\mu{}^\rho T_\rho{}^\nu&=\delta_\mu{}^\nu(\tfrac{1}{4}\Omega^2+\Lambda^2) \\ &=\tfrac{1}{4}\delta_\mu{}^\nu|\chi^2|^2, \end{aligned} \tag{III.7}$$

where

$$\begin{aligned} \Omega&=\tfrac{1}{2}\phi^{\mu\nu}\phi_{\mu\nu} \\ \Lambda&=\tfrac{1}{4}f^{\mu\nu}\phi_{\mu\nu} \\ f^{\mu\nu}&=\tfrac{1}{2}\epsilon^{\mu\nu\alpha\beta}\phi_{\alpha\beta}. \end{aligned}$$

Furthermore

$$\tfrac{1}{4}\Omega^2+\Lambda^2=[\tfrac{1}{2}(E^2+H^2)]^2-(\mathbf{E}\times\mathbf{H})^2, \tag{III.8}$$

where we took

$$\phi_{4i}=E_i, \quad H_i=\tfrac{1}{2}\epsilon_{ijk}\phi_{jk}.$$

A comparison of Eq. (III.8) with the square of a momentum vector p_μ of a particle suggests that there exists a Lorentz covariant representation of energy and momentum properties corresponding to a field $\phi_{\mu\nu}$. Thus if we take

$$p_\mu=c^{-1}T_{\mu\nu}V^\nu, \tag{III.9}$$

then we obtain

$$c^2p^\mu p_\mu=T_{\mu\rho}V^\rho T^{\mu\sigma}V_\sigma=\delta_\sigma{}^\rho V_\rho V^\sigma(\tfrac{1}{4}\Omega^2+\Lambda^2)=\tfrac{1}{4}\Omega^2+\Lambda^2,$$

where V_μ is a unit vector

$$V_\mu V^\mu=1.$$

The vector p_μ defined by Eq. (III.9) reduces, for $V_i=0$, to the usual definitions for p_4 as energy density $\frac{1}{2}(E^2+H^2)$ and p_i as momentum density $\mathbf{E}\times\mathbf{H}$.

The complex space representation of p_μ and $T_{\mu\nu}$ can be obtained, by inspection, as

$$p_\mu=(1/2c)\langle\chi|B_{\mu\nu}V^\nu|\chi\rangle, \tag{III.10}$$

$$T_{\mu\nu}=\tfrac{1}{2}\langle\chi|B_{\mu\nu}|\chi\rangle, \tag{III.11}$$

where the 10 3×3 matrices $B_{\mu\nu}$ are given by

$$\begin{aligned} &B_{44}=K_4=I_3, \quad B_{4i}=B_{i4}=K_i \\ &B_{ij}=B_{ji}=K_iK_j+K_jK_i-I_3\delta_{ij}, \end{aligned} \tag{III.12}$$

and, like $T_{\mu\nu}$ itself, they satisfy the trace property

$$a^{\mu\nu}B_{\mu\nu}=0. \tag{III.13}$$

For $V_i=0$, the vector p_μ defined by Eq. (III.10) reduces to

$$p_\mu=(1/2c)\langle\chi|K_\mu|\chi\rangle. \tag{III.14}$$

All B matrices are Hermitian and B_i and $B_{4i}=K_i$ satisfy

$$\begin{aligned} B_1{}^2+B_2{}^2+B_3{}^2&=2I_3, \\ K_1{}^2+K_2{}^2+K_3{}^2&=2I_3. \end{aligned} \tag{III.15}$$

[3] This type of equation was first discussed by J. R. Oppenheimer [Phys. Rev. **38**, 725 (1931)], and more recently W. J. Archibald [Can. J. Phys. **33**, 565 (1955)] and R. H. Good [Phys. Rev. **105**, 1914 (1957)] have investigated further quantum-mechanical implications of such an equation. Four-dimensional representations have been discussed by H. E. Moses [Nuovo cimento. Suppl. 7, 1 (1958)]; see also J. S. Lomont, Phys. Rev. **111**, 1710 (1958).

The K matrices as spin-1 matrices satisfy the usual commutation relations

$$K_iK_j-K_jK_i=i\epsilon_{ijl}K_l. \tag{III.16}$$

IV. TIME REVERSAL AND ANTIORTHOGONAL TRANSFORMATIONS

The transformation properties of B matrices under Lorentz transformations can be derived from the vector and tensor transformation properties of p_μ and $T_{\mu\nu}$ as defined by Eqs. (III.10) and (III.11), respectively.

The tensor $T_{\mu\nu}$ in another Lorentz frame has the form

$$T_{\mu\nu}'=\tfrac{1}{2}\langle\chi'|B_{\mu\nu}|\chi'\rangle, \tag{IV.1}$$

where $|\chi'\rangle$ is a function of the new coordinates x_μ' related to the old coordinates x_μ by a Lorentz transformation

$$|x')=L|x), \tag{IV.2}$$

where L is a Lorentz matrix satisfying

$$\tilde{L}FL=F, \tag{IV.3}$$

and $|x)$ is the column vector of the coordinates and time. The ket $|\chi'\rangle$ is transformed by an R transformation, according to

$$|\chi'\rangle=R|\chi\rangle. \tag{IV.4}$$

Application of these transformations to Eq. (IV.1) and the requirement that transformations should hold for all vectors of complex space, yield the transformation rules of B matrices,

$$R^\dagger B_{\mu\nu}R=L_\mu{}^\alpha L_\nu{}^\beta B_{\alpha\beta}. \tag{IV.5}$$

The R matrix is a function of the coefficient $L_\mu{}^\alpha$ alone. For proper R and L transformations there exist an isomorphism between L and R matrices satisfying Eq. (IV.5). The Lorentz matrices corresponding to R_1, R_2, and R_3 [see Eq. (II.15)], are given by

$$L_1(\psi,\lambda),\quad L_2(\phi,\epsilon),\quad L_3(\sigma,\rho),$$

corresponding to rotations and velocity transformations for x_1, x_2, x_3 directions, respectively.

The symmetry properties of the complex space are of great physical interest. We shall study some of these properties by the application of the improper Lorentz transformations corresponding to Lorentz matrices F, $-F$, and $-I_4$. Now, F and $-F$ correspond to space and time reflection transformations of coordinates, respectively. In complex space, the corresponding transformations can be obtained by replacing the coefficients $L_\mu{}^\alpha$ of the Lorentz matrix L by $a_\mu{}^\alpha$, leading to

$$R^\dagger B_{\mu\nu}R=a_\mu{}^\alpha a_\nu{}^\beta B_{\alpha\beta}. \tag{IV.6}$$

Hence various B matrices transform according to

$$R^\dagger R=I \tag{IV.7}$$

$$R^\dagger K_iR=-K_i \tag{IV.8}$$

$$R^\dagger B_{ij}R=B_{ij}. \tag{IV.9}$$

We shall study five different R transformations satisfying Eqs. (IV.7)–(IV.9).

(i) The R transformation corresponding to the F metric in Lorentz space can be taken to be the parity operator $\mathcal{P}$ which is a linear unitary space reflection operator and transforms the B matrices according to

$$\mathcal{P}^2=I \tag{IV.10}$$

$$\mathcal{P}^{-1}K_i\mathcal{P}=-K_i \tag{IV.11}$$

$$\mathcal{P}^{-1}B_{ij}\mathcal{P}=B_{ij}. \tag{IV.12}$$

In accordance with the c-number theory, the parity operator $\mathcal{P}$ acts on a ket $|\chi\rangle$ to produce another $|\chi'\rangle$, as

$$|\chi'\rangle=\mathcal{P}|\chi\rangle=-|\chi^*(-\mathbf{r},t)\rangle=-\bar{C}|\chi(-\mathbf{r},t)\rangle. \tag{IV.13}$$

The matrices B_{ij} remain unchanged under parity operation.

(ii) The fact that the elements of K matrices and B_{ij} matrices are pure imaginary and real numbers, respectively, suggest to choose R to be the antilinear operation of complex conjugation,

$$R=\pm\bar{C}, \tag{IV.14}$$

which satisfies Eqs. (IV.7)–(IV.9). We must, of course, note that $\mathcal{P}$ and $-\bar{C}$ operations on a ket $|\chi\rangle$ are not equivalent operations, since the former, in addition to complex conjugation, replaces $\chi(\mathbf{r},t)$ by $\chi(-\mathbf{r},t)$.

The antilinear operator $\bar{C}$ can be regarded as the "metric" of the complex space and in this sense it corresponds to the Lorentz metric F of Lorentz space.[4] We may now use the ordinary ket notation and define the scaler product of two complex vectors, without the necessity of introducing two types of scaler products, by

$$\langle\chi|\bar{C}|\chi\rangle=\chi_i{}^*\chi_i{}^*, \tag{IV.15}$$

where the effect of the antilinear operator $\bar{C}$ is to replace the expression following it by its complex conjugate. We can also define an antilinear operator $\bar{C}_L$ whose effect is to replace the expression preceding it by its complex conjugate. Thus if b is a complex number, then

$$\bar{C}b=b\bar{C}_L=b^*,$$

and

$$\bar{C}b\bar{C}_L=b\bar{C}_L{}^2=b^*\bar{C}_L=b;$$

hence

$$\bar{C}_L{}^2=1. \tag{IV.16}$$

[4] The situation here is, in some sense, similar to the metrical correspondences of the two-dimensional spinor space with metric $i\sigma_2$ and four-dimensional spinor space with metric β, to Lorentz metric F.

The scalar product of $|\chi\rangle$ with itself with respect to $\bar{C}_L$ is

$$\langle\chi|\bar{C}_L|\chi\rangle=\chi_i\chi_i.$$

The vector $\langle\chi|\bar{C}_L=\langle\chi^*|=(\chi|$ is called the adjoint of $|\chi\rangle$.

(iii) The R transformation corresponding to the coordinate time reflecting $(-F)$ Lorentz matrix can be taken as the time-reversal operator of the complex space.

A general form of the time reversal operator which can operate on vectors of the form $e^{i\delta}|\chi\rangle$ is

$$\mathcal{T}=e^{i\delta}I_3\bar{C}, \tag{IV.17}$$

and it satisfies

$$\mathcal{T}^2=1. \tag{IV.18}$$

The operator $\mathcal{T}$ as defined by Eq. (IV.17) for $\delta=0$, $\delta=\pi$, and $\delta=2\pi$ is complex orthogonal and for $\delta=\frac{1}{2}\pi$ is an antiorthogonal operator;

$$\begin{aligned}&\tilde{\mathcal{T}}\mathcal{T}=I \quad \text{for} \quad \delta=0,\pi,2\pi\\ &\tilde{\mathcal{T}}\mathcal{T}=-I \quad \text{for} \quad \delta=\tfrac{1}{2}\pi.\end{aligned} \tag{IV.19}$$

The K matrices under time-reversal operation transform as

$$\tilde{\mathcal{T}}K_i\mathcal{T}=-K_ie^{2i\delta}, \tag{IV.20}$$

and

$$\mathcal{T}^{-1}K_i\mathcal{T}=-K_i. \tag{IV.21}$$

For $\delta=\frac{1}{2}\pi$ the parity transformation (IV.11) and the time-reversal transformation (IV.20) prove that K_i transform like a polar, as well as an axial, vector. The vector iK_i behaves differently under $\mathcal{T}$ transformation, since

$$\tilde{\mathcal{T}}iK_i\mathcal{T}=iK_ie^{-2i\delta}, \tag{IV.22}$$

and

$$\mathcal{T}^{-1}iK_i\mathcal{T}=iK_i, \tag{IV.23}$$

so that iK_i for $\delta=\frac{1}{2}\pi$ behaves like an axial vector.

(iv) Lorentz transformation reflecting both space and time coordinates is affected by $-L_4$ and corresponding transformation of B matrices reduce to

$$R^\dagger B_{\mu\nu}R=B_{\mu\nu},$$

or

$$R^\dagger R=I, \quad R^\dagger K_iR=K_i, \quad R^\dagger B_{ij}R=B_{ij}. \tag{IV.24}$$

These equations are satisfied by the successive application of time reversal and space-reflection operators. Thus the R transformation in complex space, corresponding to simultaneous reflection of space and time coordinates in Lorentz space, can be represented as

$$R=\mathcal{T}\mathcal{P}=e^{i\delta}\bar{C}\mathcal{P}. \tag{IV.25}$$

This also for $\delta=\frac{1}{2}\pi$ is an antiorthogonal transformation.

(v) Simultaneous reflection of space, time, and field can be affected by the transformation operator

$$R=-e^{i\delta}\bar{C}\mathcal{P}. \tag{IV.26}$$

V. TWO-VALUED REPRESENTATION OF COMPLEX GROUP

The invariance requirement of Eq. (II.2) can be represented by a similarity transformation,

$$F'=U^{-1}GU, \tag{V.1}$$

where

$$G=i\begin{bmatrix}\chi_3 & \chi_-\\ \chi_+ & -\chi_3\end{bmatrix}$$

$$G'=i\begin{bmatrix}\chi_3' & \chi_5'\\ \chi_+' & -\chi_3'\end{bmatrix}$$

$$\chi_\pm=\chi_1\pm i\chi_2.$$

The factor i in the definition of G, as will be seen later, is needed for invariance reasons. The 2×2 complex matrix U is subject to the condition

$$\det U=1, \tag{V.2}$$

which provide two equations among the four complex elements of U. Thus U matrices can constitute a two-valued six parameter representation of the complex orthogonal group. The determinant of Eq. (V.1) is

$$\chi_1'^2+\chi_2'^2+\chi_3'^2=\chi_1^2+\chi_2^2+\chi_3^2. \tag{V.3}$$

Furthermore, in terms of Pauli matrices, Eq. (V.1) can be written as

$$i\boldsymbol{\sigma}\cdot\boldsymbol{\chi}'=U^{-1}i\boldsymbol{\sigma}\cdot\boldsymbol{\chi}U, \tag{V.4}$$

where the factor i on both sides of the equation, because of the possible antilinear U operations, cannot be canceled out.[5]

Under a Lorentz transformation of coordinate the ket $|\chi(x)\rangle$ will be transformed by the corresponding R matrix according to $|\chi'\rangle=R|\chi\rangle$ and correspondingly a two-component ket $|u\rangle$ of the spinor space will be transformed by the corresponding U matrix according to

$$|u'\rangle=u|U\rangle. \tag{V.5}$$

[5] The two-dimensional spinor space under consideration here is, in some respects, quite different from the two-dimensional spinor space where one considers the transformation properties of the vector matrix $\sigma_\mu=(\sigma_i,\sigma_4=I_2)$. In the former space the condition $\det U=1$ is not a necessity and the U transformations are directly determined from R transformations. In the latter spinor space the transformation laws of σ_μ are given by

$$S^\dagger\sigma_\mu S=L^\nu{}_\mu\sigma_\nu,$$

where the condition $\det S=1$ is a necessity and S are defined directly in terms of the coefficients $L_\mu{}^\alpha$. Also well-known properties of σ_μ under improper Lorentz transformations draws a sharp line of demarcation between U and S transformations. The said reasons and others, to be discussed in later sections, will allow us to regard U and R transformations as charge space representations of Lorentz group. In particular, for quantized $|\chi\rangle$ the operators

$$T_i=\tfrac{1}{2}\int\langle\chi|K_i|\chi\rangle d^3r$$

may be related to the representation of the isotopic spin group, where χ has an additional isotopic spin coordinate referring to three charge states.

On replacing χ_i' in Eq. (V.4) by

$$\chi_i' = R_{ij}\chi_j, \tag{V.6}$$

and noting that Eq. (V.4) must hold for all proper R transformations of the complex space, we obtain

$$i\sigma_i R_{ij} = U^{-1} i\sigma_j U \tag{V.7}$$

as the transformation rules of σ's. The U matrix is a function of the coefficients R_{ij} alone.

It can easily be verified that the six-parameter group of U matrices

$$\begin{aligned} U_1 &= \pm\exp[(-i\tfrac{1}{2}\psi + \tfrac{1}{2}\lambda)\sigma_1] \\ U_2 &= \pm\exp[(-\tfrac{1}{2}i\phi + \tfrac{1}{2}\epsilon)\sigma_2] \\ U_3 &= \pm\exp[(-i\tfrac{1}{2}\theta + \tfrac{1}{2}\rho)\sigma_3], \end{aligned} \tag{V.8}$$

together with R matrices given by Eq. (II.15) satisfy[6] Eq. (V.7).

To find the U transformations corresponding to improper and antiorthogonal R transformations it is, because of the antilinear operations involved, necessary to use Eq. (V.4) instead of Eq. (V.7). Since parity operation is not an invariant transformation in the two-component spinor space, we need not consider the case $R=\mathcal{P}$.

For $R=\bar{C}$ from Eq. (V.4) we obtain

$$i\sigma_i\chi_i^* = U^{-1} i\sigma_i \chi_i U, \tag{V.9}$$

which, obviously, implies an antilinear U operation. Let us put

$$U = \Gamma\bar{C},$$

where Γ is a 2×2 matrix to be calculated. From Eq. (V.9) we can write

$$\begin{aligned} i\sigma_i\chi_i^* &= (\bar{C})^{-1}\Gamma^{-1} i\sigma_i\chi_i\Gamma\bar{C} = \bar{C}\Gamma^{-1} i\sigma_i\chi_i\Gamma\bar{C} \\ &= -(\Gamma^*)^{-1} i\sigma_i{}^L\chi^*{}_i\Gamma^*. \end{aligned}$$

The special matrix $f = i\sigma_2$ transforms σ's according to

$$f^{-1}\sigma_i f = -\sigma_i{}^L, \tag{V.10}$$

where $\sigma_i{}^L$ are left-handed Pauli matrices (which differ from the normal ones only in the sign of σ_2) and $f^2=-1$. Thus we may conveniently choose $\Gamma = f$ and obtain

$$i\sigma_i\chi_i^* = -f^{-1} i\sigma_i{}^L\chi_i^* f = i\sigma_i\chi_i^*.$$

Hence the required antilinear U transformation (up to an arbitrary phase factor) is

$$U = T = f\bar{C}, \tag{V.11}$$

where $\mathcal{T}$ satisfies

$$\mathcal{T}^2 = -1. \tag{V.12}$$

Transformations of $i\sigma_i$ and σ_i under T are

$$\mathcal{T}^{-1} i\sigma_i \mathcal{T} = i\sigma_i, \tag{V.13}$$

and

$$\mathcal{T}^{-1}\sigma_i\mathcal{T} = -\sigma_i. \tag{V.14}$$

One can also define a left operator T_L by

$$\mathcal{T}_L = \bar{C}_L f. \tag{V.15}$$

The time-reversal operator $\mathcal{T}$ defined by Eq. (V.11) for the two-dimensional spinor space is well known. The only result here is its correspondence to the time reversal operator $R=\bar{C}$ (for $\delta=0$) of the complex space.

VI REPRESENTATION OF PROPER COMPLEX GROUP

For the sake of completeness we first give a sketch of the concept of infinitesimal transformation of the complex space. For a given generator $Z(\tau)$ we can regard Eq. (II.12) as an equation describing time development of the transformation operator R from the identity operator I_3 at an initial time τ_0. In this case Eq. (II.12) can be replaced by the integral equation

$$R(\tau,\tau_0) = I_3 - i\int_{\tau_0}^{\tau} \epsilon_+(\tau,\tau_1)Z(\tau_1)R(\tau_1,\tau_0)d\tau_1, \tag{VI.1}$$

where $\epsilon_+(\tau,\tau_1)=1$ for $\tau \geqq \tau_0$ and it is zero for $\tau<\tau_0$. The function ϵ_+ incorporates the direction of the flow of time ($\tau>\tau_0$) into the integral equation (VI.1).

The integral equation (VI.1), from group theoretical point of view, is most suitable for a consistent discussion of infinitesimal transformations. If we assume that $Z(\tau)$ is a continuous function of time in the interval (τ_0,τ) then it is quite easy to prove, by means of the boundedness of the norm of $Z(\tau)$, that the integral equation (VI.1) has a well-defined solution. A symbolic form of the solution is

$$R(\tau,\tau_0) = P\exp\left[-i\int_{\tau_0}^{\tau_1} Z(\tau_1)d\tau_1\right], \tag{VI.2}$$

where P is an operator for time labeling of the products of operators.[7]

The result (VI.2) for complex transformation operators can, of course, be obtained for Lorentz transformation matrices also, as

$$L(\tau,\tau_0) = P\exp\left[-i\int_{\tau_0}^{\tau} A(\tau_1)Fd\tau_1\right], \tag{VI.3}$$

where $A(\tau_1)$ is a 4×4 Hermitian and antisymmetric matrix.

For a time-independent generator Z, the infinitesimal complex rotation operator is given by

$$R = I_3 - iZ. \tag{VI.4}$$

[6] Actually if we wished we could set up the said one-two correspondence of R and U transformations as one-two correspondence of rotations and velocity transformations separately. For example, the rotation and velocity transformations of the complex space affected by the R matrices $R_i(\theta_i)=\exp(i\theta_i K_i)i$ $=1,2,3$ (not summed over i) and $R_i(\rho_i)=\exp(-\rho_i K_i)$ correspond to rotations and velocity transformations of the spinor space affected by the U matrices

$$U_i(\tfrac{1}{2}\theta_i) = \pm\exp(-\tfrac{1}{2}i\theta_i\sigma_i)$$

and

$$U_i(\tfrac{1}{2}\rho_i) = \pm\exp(\tfrac{1}{2}\rho_i\sigma_i),$$

respectively.

[7] F. J. Dyson, Phys. Rev. **75**, 486 (1949).

Also from Eq. (VI.3) the infinitesimal Lorentz transformation matrix is

$$L=I_4-iAF,$$

or

$$L_\mu{}^\nu=\delta_\mu{}^\nu-\omega_\mu{}^\nu, \tag{VI.5}$$

where

$$\omega_{\mu\nu}=-\omega_{\nu\mu}.$$

By using the transformation rules (IV.5), relating R and L transformations, we can express the Z operator in terms of the infinitesimal coefficients $\omega_{\mu\nu}$ by

$$Z=i\boldsymbol{\varepsilon}\cdot\mathbf{K}+\boldsymbol{\omega}\cdot\mathbf{K}, \tag{VI.6}$$

where

$$\omega_{4i}=\epsilon_i, \quad \omega_2=\tfrac{1}{2}\epsilon_{ijf}\omega_{ij}.$$

The total change in a ket $|\chi\rangle$ under an infinitesimal Lorentz transformation as a combined effect of R and L transformations can be expressed as

$$\Delta|\chi\rangle=|\chi'(x)\rangle-|\chi(x)\rangle=-\frac{i}{\hbar}(\boldsymbol{\omega}\cdot\mathbf{J})|\chi\rangle + \left[\boldsymbol{\varepsilon}\cdot\mathbf{K}+\frac{i}{\hbar}\epsilon_i(x^4p_i-x^ip_4)\right]|\chi\rangle, \tag{VI.7}$$

where we used the representation $p_\mu=-i\hbar(\partial/\partial x^\mu)$ and

$$\mathbf{J}=\mathbf{L}+\hbar\mathbf{K} \tag{VI.8}$$

is the total angular-momentum operator of the electromagnetic field. It satisfies the usual angular momentum commutation rules

$$[J_i,J_j]=i\hbar\epsilon_{ijl}J_l, \tag{VI.9}$$

and

$$[J^2,J_i]=0. \tag{VI.10}$$

Moreover, the operator J commutes with the "Hamiltonian" operator

$H=c\mathbf{K}\cdot\mathbf{p}$, Eq. (III.5) of the electromagnetic field,

$$[J_i,H]=0, \tag{VI.11}$$

which means that if $|\chi\rangle$ is a solution of Maxwell's equations, then the ket

$$|\chi_J\rangle=(\boldsymbol{\omega}\cdot\mathbf{J})|\chi\rangle \tag{VI.12}$$

is also a solution.

It follows from the preceding expressions that the proper irreducible representations of the complex orthogonal group can be derived via Maxwell's equations (III.4). All these representations can be expressed as vector spherical harmonics.

Derivation of the double-valued representations, together with the proper representations, can proceed from the commutation rules (VI.10) and (VI.9) in the usual way.

VII. FOUR-DIMENSIONAL REPRESENTATION OF COMPLEX GROUP

Various symmetry operations in spinor fields (time reversal, space inversion, charge conjugation, etc.) can be studied as operations induced by the complex representations of Lorentz group. Electromagnetic concept of charge can be used to describe charge conjugation in complex space as a special gauge transformation which consists of a trivial linear operation of multiplication of $|\chi\rangle$ by -1. Thus, charge conjugation operation in complex space belongs to the extended complex group and is not the same as $\mathcal{PT}$ operation in complex space. Charge conjugation will not be discussed in this paper.

In order to bring about the main features of the representation, it is convenient to consider the transformation properties of a spinor $|\phi\rangle$ defined by

$$|\phi\rangle=\gamma^\mu p_\mu|\psi\rangle, \tag{VII.1}$$

where $|\phi\rangle$ and $|\psi\rangle$ are four-component spinor functions of space and time. We choose the representation of Dirac matrices where γ_i (i=1,2,3) are Hermitian and $\gamma_4=i\beta$ is anti-Hermitian and they satisfy the anti-commutation relations

$$\gamma_\mu\gamma_\nu+\gamma_\nu\gamma_\mu=-2a_{\mu\nu}I_4. \tag{VII.2}$$

The four-vector p_μ is defined by Eq. (III.10), so that Eq. (VII.1) will be written as

$$|\phi\rangle=(1/2c)\langle\chi|B_{\mu\nu}V^\nu|\chi\rangle\gamma^\mu|\psi\rangle. \tag{VII.3}$$

Under a Lorentz transformation of coordinates,

$$|x'\rangle=L|x\rangle, \tag{VII.4}$$

the spinor $|\psi\rangle$ (and $|\phi\rangle$) and the complex vector $|\chi\rangle$ are transformed according to

$$|\psi'\rangle=S|\psi\rangle \tag{VII.5}$$

$$|\chi'\rangle=R|\chi\rangle, \tag{VII.6}$$

where S is the transformation operator of the four-dimensional spinor space corresponding to R. Using the transformations (VII.4)–(VII.6) in Eq. (VII.3), we obtain (in the usual way)

$$R^\dagger B_{\mu\nu}R\gamma^\nu=L_\mu{}^\rho B_{\rho\nu}S\gamma^\nu S^{-1}, \tag{VII.7}$$

for all complex vectors $|\chi\rangle$, spinors $|\psi\rangle$, and unit vectors V_μ. The expressions (VII.7) for a given Lorentz matrix L relate R transformations of complex space to the S transformations of spinor space and they are based on the Lorentz covariance requirement of a particular spinor $|\phi\rangle$ defined by Eq. (VII.3). A typical set of proper transformations satisfying Eq. (VII.7) are

$$L=\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & \cos\psi & \sin\psi & 0\\ 0 & -\sin\psi & \cos\psi & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$$

$$R=\exp[-i\psi K_1] \tag{VII.8}$$

$$S=\exp[-\tfrac{1}{2}\psi\gamma_2\gamma_3],$$

corresponding to rotations in Lorentz space, complex space, and spinor space, respectively.

We shall be interested in the isomorphism of the representations of Lorentz group by L, R, and S matrices for various linear and antilinear symmetry operations.

(i) Space inversion: The Lorentz transformation (of class $L_{44}\geqq 1$) $L_\nu{}^\mu=a_\nu{}^\mu$ substituted in Eq. (VII.7) yields

$$R^\dagger R\gamma^4+R^\dagger K_i R\gamma^i=S\gamma^4S^{-1}+K_iS\gamma^iS^{-1}, \quad \text{(VII.9)}$$

and

$$R^\dagger K_i R\gamma^4+R^\dagger B_{ij}R\gamma^i=-K_iS\gamma^4S^{-1}-B_{ij}S\gamma^iS^{-1}. \quad \text{(VII.10)}$$

It is easily seen from these equations that the operation $R=\mathcal{P}$ in complex space corresponds to the operation $S=\exp(i\lambda)\beta$ in spinor space, where λ is a constant. If $|\psi\rangle$ is regarded as a state vector, then, as is well known, the parity transformation for spinors is

$$\mathcal{P}|\psi(x,t)\rangle=\exp(i\lambda)\beta|\psi(-x,t)\rangle,$$

so that we must have

$$\exp(2i\lambda)=1,$$

or $\lambda=0$ and $\lambda=\pi$. Hence S is equivalent to an operation by $\pm\beta$ plus reflection of space. If only $R=\pm\bar{C}$ is considered, then the corresponding S operation is just $\pm\beta$ on $|\psi\rangle$.

(ii) Time reversal: With the Lorentz transformation matrix $L_\nu{}^\mu=-a_\nu{}^\mu$ (class $L_{44}\leqq -1$) Eq. (VII.7) reduce to

$$R^\dagger R\gamma^4+R^\dagger K_i R\gamma^i=-S\gamma^4S^{-1}-K_iS\gamma^iS^{-1},$$

and

$$R^\dagger K_i R\gamma^4+R^\dagger B_{ij}R\gamma^i=K_iS\gamma^4S^{-1}+B_{ij}S\gamma^iS^{-1}. \quad \text{(VII.11)}$$

Hence the antiorthogonal time-reversal operation, $\mathcal{T}=e^{i\delta}I_3\bar{C}$ on a ket $|\chi\rangle$ in complex space, corresponds to the operation $S=\beta\gamma_5$ plus the operation of complex conjugation on the spinor $|\psi\rangle$, where

$$\gamma_5=\gamma_1\gamma_2\gamma_3\gamma_4=\begin{bmatrix}0 & iI_2\\ iI_2 & 0\end{bmatrix}.$$

Time-reversal operation on $|\psi\rangle$, regarded as a state vector, is

$$\mathcal{T}|\psi\rangle=\beta\gamma_5\bar{C}|\psi\rangle, \quad \text{(VII.12)}$$

where $\mathcal{T}$ satisfies

$$\mathcal{T}^2=-1 \quad \text{(VII.13)}$$

for a single spin-$\frac{1}{2}$ particle state.

(iii) Weak reaction[8]: In this case the Lorentz transformation matrix is $L_\nu{}^\mu=-\delta_\nu{}^\mu$ (class $L_{44}\leqq -1$) and R and L transformations are related by

$$R^\dagger B_{\mu\nu}R\gamma^\nu=-B_{\mu\nu}S\gamma^\nu S^{-1}, \quad \text{(VII.14)}$$

or

$$\begin{aligned}&R^\dagger R\gamma^4+R^\dagger K_i R\gamma^i=-S\gamma^4S^{-1}-K_iS\gamma^iS^{-1}\\ &R^\dagger K_i R\gamma^4+R^\dagger B_{ij}R\gamma^i=-K_iS\gamma^4S^{-1}-B_{ij}S\gamma^iS^{-1}.\end{aligned} \quad \text{(VII.15)}$$

Weak reflection in complex space results from a successive application of time reversal and space-reflection operation as

$$R=\mathcal{T}\mathcal{P}=e^{i\delta}\bar{C}P.$$

The corresponding weak reflection operation in spinor space is obtained in the same way as

$$S=(\pm\beta)(\beta\gamma_5)=\pm\gamma_5. \quad \text{(VII.16)}$$

The R and S defined in this way satisfy Eq. (VII.15). The symmetry operation by $\mathcal{T}\mathcal{P}$ in complex space on $|\chi\rangle$ corresponds to the symmetry operation

$$S|\psi\rangle=\pm\gamma_5\bar{C}|\psi\rangle \quad \text{(VII.17)}$$

in spinor space on $|\psi\rangle$.

(iv) Strong reflection: For the complex space the operation of strong reflection results from the multiplication by -1 (change of the sign of the field) of the weak reflection operation, viz.,

$$R=-e^{i\delta}\bar{C}\mathcal{P}, \quad \text{(VII.18)}$$

which on operating on $e^{i\delta}|\chi\rangle$ yields

$$Re^{i\delta}|\chi(x)\rangle=|\chi(-x)\rangle. \quad \text{(VII.19)}$$

The corresponding strong reflection for spinor space and relevance of the complex representation to the discussion of spin and statistics will be made the subject matter of another paper.

The results of the foregoing sections lead to the symmetry operations given in Table I.

TABLE I.

Lorentz group	Space reflection	Time reversal	Weak reflection
Complex representation	$\mathcal{P}$	$e^{i\delta}\bar{C}$	$e^{i\delta}\bar{C}\mathcal{P}$
Two-dimensional representation		$f\bar{C}$	
Four-dimensional representation	$\pm\beta\mathcal{P}$	$\beta\gamma_5\bar{C}$	$\pm\gamma_5\bar{C}$

The three symmetry operations $\mathcal{P}$, $e^{i\delta}\bar{C}$, and $e^{i\delta}\bar{C}\mathcal{P}$ of the complex group together with the unit operation I_3 form a group. The product of the three operations is the identity element I_3 of the group.

VIII. CHARGE SPACE

The following is a preliminary discussion of the possibility of relating electromagnetic concept of charge to the complex representation of Lorentz group. In particular, representation of a chargeless state by a complex wave function does not seem to present any formal or conceptual difficulties. Also a Majorana

[8] The symmetry operation of weak reflection here is not used in the sense introduced by Pauli [*Niels Bohr and the Development of Physics* (Pergamon Press, New York, 1955)] who defined it as a combination of two symmetry operations of (i) reflection of space time coordinates together with transformation of every particle into its antiparticle (strong reflection) and (ii) particle, antiparticle conjugation. Similar considerations by J. Schwinger were given in Phys. Rev. **82**, 914 (1951), and also by G. Luders, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **28**, No. 5 (1954). A different approach to a complex four-dimensional representation of Lorentz group is given by Res. Yost, Helv. Phys. Acta. **30**, 407 (1957).

neutrino does not fit into the scheme of complex representation. We shall discuss only the c-number theory.[9]

We begin by the simple observation that the fundamental invariant of the complex space,

$$Q^2=\chi_1^2+\chi_2^2+\chi_3^2=\langle\chi|\bar{C}_L|\chi\rangle, \qquad \text{(VIII.1)}$$

and its complex conjugate,

$$Q^{*2}=\chi_1^{*2}+\chi_2^{*2}+\chi_3^{*2}=\langle\chi|\bar{C}|\chi\rangle, \qquad \text{(VIII.2)}$$

will vanish for a plane electromagnetic wave. Let us assume that the vanishing of Q^2 corresponds to an invariant statement of zero charge for a massless field. The invariant Q^{*2}, with respect to the point $Q^2=0$, is to be regarded as the image of Q^2 in a space consisting of three points 0, Q^2, Q^{*2} (charge space). The complex invariant quantity Q is related to electric charge in some abstract way which will be somewhat clarified by considering the correspondence between photon and neutrino as implied by the complex group.

The functional relationship between the points Q^2 and Q^{*2} is such that they are situated from the point $Q^2=0$ and from one another at "invariant distances." The points Q^2 and Q^{*2}, being related by an antilinear transformation, cannot be transformed into one another by means of a linear unitary transformation. Under R transformations the "charge lattice" $(0,Q^2,Q^{*2})$ remains an invariant structure of the charge space. A more general charge space can be defined by including gauge group in the complex group (extended group).

Two important linear operators related to charge space can be obtained from adding and subtracting Eqs. (VIII.1) and (VIII.2), as

$$\tfrac{1}{2}(Q^2+Q^{*2})=\langle\chi|Y|\chi\rangle=\Omega, \qquad \text{(VIII.3)}$$

and

$$\tfrac{1}{2}(Q^2-Q^{*2})=\langle\chi|X|\chi\rangle=-2i\Lambda, \qquad \text{(VIII.4)}$$

where

$$Y=\tfrac{1}{2}(\bar{C}+\bar{C}_L), \qquad \text{(VIII.5)}$$

$$X=\tfrac{1}{2}(\bar{C}-\bar{C}_L), \qquad \text{(VIII.6)}$$

are linear (!) Hermitian and anti-Hermitian operators, respectively. The operators Y and X satisfy the algebraic equations

$$Y^3=Y \qquad \text{(VIII.7)}$$

$$X^3=X. \qquad \text{(VIII.8)}$$

Thus both Y and X have eigenvalues $+1$, -1, and 0. The effects of Y and X on a complex number b are

$$[Y,b]=[b^*,Y], \qquad \text{(VIII.9)}$$

and

$$[X,b]_+=[b^*,X]_+. \qquad \text{(VIII.10)}$$

[9] For a q-number theory the field χ_i must be quantized according to

$$[\chi_i^*,\chi_j]=iR_F,$$

where

$$R_F=[i\hbar(\partial/\partial t)+H]D_F(x-x'),$$

and D_F is the usual propagator of electromagnetic field.

Both Y and X belong to the complex representation of the complex group.

The effect of the linear unitary operator $\bar{C}\bar{C}_L$ can be seen by writing the Hermitian scalar product of two complex vectors $|\chi\rangle$ and $|\eta\rangle$

$$\langle\eta|\chi\rangle=\langle\chi|\bar{C}_L\bar{C}|\eta\rangle=(\langle\chi|\eta\rangle)^\dagger. \qquad \text{(VIII.11)}$$

Hence we see that the action of the operator $\bar{C}\bar{C}_L$ consists of operation of complex conjugation plus transposition.

The usual geometrical analysis for the representation of the proper rotations of three-dimensional Euclidean space about the origin of Cartesian coordinates can be generalized for application in complex domain where the coordinates are replaced by complex functions of space and time. We first discuss the most general form of stereographic projection of a unit sphere about the origin on to the equatorial plane $x_3=0$, with the south pole as the center of projection. To the point x_1, x_2, x_3 on the sphere corresponds the point x_1', x_2', 0 on the plane and the formulas for the projection are

$$x_1+ix_2=2a/(1+aa^*)=x_+$$

$$x_1-ix_2=2a^*/(1+aa^*)=x_-$$

$$x_3=(1-aa^*)/(1+aa^*),$$

where

$$a=x_1'+ix_2'=u_2/u_1,$$

and u_1, u_2 are homogeneous complex coordinates which enables us to include the south pole of the sphere in the projection. In terms of the coordinates u_1 and u_2 we have

$$x_+=\frac{2u_1^*u_2}{|u_1|^2+|u_2|^2},\quad x_-=\frac{2u_1u_2^*}{|u_1|^2+|u_2|^2},\quad x_3=\frac{|u_1|^2-|u_2|^2}{|u_1|^2+|u_2|^2}.$$

Let us, now, put

$$d_2=\begin{bmatrix}-x_+ & x_3\\ x_3 & x_-\end{bmatrix},$$

where

$$\det d_2=-(x_1^2+x_2^2+x_3^2)=-1.$$

By using the projection formulas we can write d_2 as

$$d_2=w^2\langle u|[(\tau\times\sigma)_2-i\tau_2]|u\rangle, \qquad \text{(VIII.12)}$$

where

$$w=(|u_1|^2+|u_2|^2)^{-\frac{1}{2}},$$

and τ matrices are of the same type as σ matrices and they commute with σ's.

The form of Eq. (VIII.12) suggests that we can complete it into a vector matrix operator

$$d_i=w^2\langle u|[(\tau\times\sigma)_i-i\tau_i|u\rangle, \qquad \text{(VIII.13)}$$

and obtain three possible projections of the point (x_1,x_2,x_3) on the unit sphere. The matrices d_1 and d_3 are given by

$$d_1=-i\begin{bmatrix}x_+ & -x_3\\ x_3 & x_-\end{bmatrix},\quad d_3=-i\begin{bmatrix}x_3 & x_-\\ -x_+ & x_3\end{bmatrix},$$

and their determinants are

$$\det d_1=\det d_2=\det d_3=-(x_1^2+x_2^2+x_3^2).$$

Thus the three possible stereographic projections represented by d_i form a vector and they satisfy

$$d_1^2+d_2^2+d_3^2=x_1^2+x_2^2+x_3^2=1,$$

so that the operators d_i lie on the unit sphere. In terms of σ and K matrices, Eq. (VIII.13) can be written as

$$d_i=-i(\sigma^\mu K_\mu)^{ij}\langle u_I|\tau_j|u_I\rangle, \qquad \text{(VIII.14)}$$

and

$$d_i=-i(\sigma^\mu K_\mu)^{ij}x_j, \qquad \text{(VIII.15)}$$

where

$$|u_I\rangle=w|u\rangle=w\begin{bmatrix}u_1\\u_2\end{bmatrix}.$$

Hence, each unitary transformation

$$|u'\rangle=U|u\rangle, \quad U^\dagger U=I$$

on the equatorial plane, i.e., the spinor plane, corresponds to a rotation of the sphere.

It is interesting to note that the operator $-i\sigma^\mu K_\mu$ is related to the projection operator

$$P_c^2=P_c,$$

where

$$P_c=\tfrac{1}{3}\sigma^\mu K_\mu. \qquad \text{(VIII.16)}$$

The spin operators

$$S_i=K_i+\tfrac{1}{2}\sigma_i \qquad \text{(VIII.17)}$$

commute with P_c. The operators S_i can operate on the products of kets of $\boldsymbol{\sigma}$-spin and $\mathbf{K}$-spin spaces.

We may, now, generalize the results to the complex space. The projection of the "complex sphere" on to a spinor plane consists of three second rank spinors which together transform like a complex vector and each one by itself is a second rank spinor. The stereographic projections of $|\chi\rangle$ are given by

$$|\zeta\rangle=-i\sigma^\mu K_\mu|\chi\rangle,$$

or

$$\begin{pmatrix}\zeta_1\\\zeta_2\\\zeta_3\end{pmatrix}=\begin{pmatrix}-iI_2 & -\sigma_3 & +\sigma_2\\+\sigma_3 & -iI_2 & -\sigma_1\\-\sigma_2 & +\sigma_1 & -iI_2\end{pmatrix}\begin{pmatrix}\chi_1\\\chi_2\\\chi_3\end{pmatrix}, \qquad \text{(VIII.18)}$$

where the spinor indices of σ's and ζ's are suppressed.

The formulas of the stereographic projections are

$$\chi_+=\frac{2Qa}{1+ab}, \quad \chi_-=\frac{2Qb}{1+ab}, \quad \chi_3=Q\frac{1-ab}{1+ab}, \qquad \text{(VIII.19)}$$

where

$$a=\chi_1'+i\chi_2', \quad b=\chi_1'-i\chi_2'.$$

Note that b is not equal to the complex conjugate of a. On putting $a=u_2/u_1$ and $b=v_2/v_1$ in Eq. (VIII.19), we obtain

$$\chi_+=\frac{2Qu_2v_1}{u_1v_1+u_2v_2},$$

$$\chi_-=\frac{2Qu_1v_2}{u_1v_1+u_2v_2}, \qquad \text{(VIII.20)}$$

$$\chi_3=Q\frac{u_1v_1-u_2v_2}{u_1v_1+u_2v_2},$$

which satisfy

$$\chi_+\chi_-+\chi_3^2=Q^2,$$

and

$$\det\begin{bmatrix}-\chi_+ & \chi_3\\ \chi_3 & \chi_-\end{bmatrix}=-Q^2.$$

The three stereographic projections are given by

$$\zeta^i=-i(\sigma^\mu K_\mu)^{ij}(v_1|\tau_j|u_I), \qquad \text{(VIII.21)}$$

where

$$(v_I|=W[v_1,v_2], \ |u_I)=W\begin{bmatrix}u_1\\u_2\end{bmatrix}, \quad W=(u_1v_1+u_2v_2)^{-\frac{1}{2}}.$$

From Eq. (VIII.18) we have

$$\zeta^1=-i\begin{bmatrix}\chi_+ & -\chi_3\\ \chi_3 & \chi_-\end{bmatrix},$$

$$\zeta^2=\begin{bmatrix}-\chi_+ & \chi_3\\ \chi_3 & \chi_-\end{bmatrix}, \qquad \text{(VIII.22)}$$

$$\zeta^3=-i\begin{bmatrix}\chi_3 & \chi_-\\ -\chi_+ & \chi_3\end{bmatrix},$$

where the ζ matrices satisfy

$$(\zeta^1)^2+(\zeta^2)^2+(\zeta^3)^2=Q^2, \qquad \text{(VIII.23)}$$

and

$$\det\zeta^1=\det\zeta^2=\det\zeta^3=-Q^2$$
$$\det(\zeta^1+\zeta^2)=\det(\zeta^2+\zeta^3)=\det(\zeta^3+\zeta^1)=-2Q^2$$
$$\det(\zeta^1+\zeta^2+\zeta^3)=-3Q^2.$$

We shall regard the equatorial plane containing E and H of the plane electromagnetic wave as the "neutral plane" of the stereographic projections. On the latter plane we have $Q^2=0$. In this case the three spinors ζ^i are equivalent. From Eq. (VIII.19) we can write

$$a^{-1}\chi_++a\chi_-=2Q$$
$$b^{-1}\chi_-+b\chi_+=2Q,$$

so that for $Q=0$ we obtain

$$a^2b^2=1 \quad \text{or} \quad (ab-1)(ab+1)=0.$$

The case $ab-1=0$ corresponds to the trivial state $\chi_1=\chi_2=\chi_3=0$. In case $ab+1=0$ the quantity

$$2Q/(ab+1)$$

must, on the basis of physics of a free electromagnetic field, remain finite for $Q=0$, $(ab+1=0)$, since otherwise χ's would be infinite for pure electromagnetic wave. For simplicity we shall take

$$\lim_{Q=0}\left(\frac{2Q}{ab+1}\right)=1 \qquad \text{(VIII.24)}$$

which can be regarded as a normalization condition on the spinors $|u\rangle$ and $|v\rangle$. Thus on the neutral plane we have, from Eq. (VIII.20), the results

$$\chi_+=u_2v_1,\quad \chi_-=u_1v_2,\quad \chi_3=\tfrac{1}{2}(u_1v_1-u_2v_2), \qquad \text{(VIII.25)}$$

subject to the condition

$$u_1v_1+u_2v_2=0,$$

or

$$v_1/u_2=-v_2/u_1=-q$$

where q is a complex number. Hence Eqs. (VIII.25) become

$$\chi_+=-qu_2^2,\quad \chi_-=qu_1^2,\quad \chi_3=-qu_1u_2,$$

and the components of the complex ket are given by

$$\begin{aligned}\chi_1&=\tfrac{1}{2}q(u_1^2-u_2^2)\\ \chi_2&=\tfrac{1}{2}iq(u_1^2-u_2^2)\\ \chi_3&=-qu_1u_2.\end{aligned} \qquad \text{(VIII.26)}$$

The vanishing of Q^2 is independent of a particular choice of the complex number q and, therefore, it can be absorbed into the spinor $|u\rangle$ and we can write Eq. (VIII.26) as

$$\begin{aligned}\chi_1&=\tfrac{1}{2}(u_1^2-u_2^2)\\ \chi_2&=\tfrac{1}{2}i(u_1^2+u_2^2)\\ \chi_3&=-u_1u_2.\end{aligned} \qquad \text{(VIII.27)}$$

By using these transformations we can express the momentum vector p_μ defined by Eq. (III.14) in terms of the two-components spinor $|u\rangle$ as

$$p_\mu=(1/2c)\langle\psi_\nu|\sigma_\mu|\psi_\nu\rangle, \qquad \text{(VIII.28)}$$

where

$$|\psi_\nu\rangle=(cp_4)^{\frac{1}{2}}|u\rangle,$$

and

$$cp_4=\tfrac{1}{2}(|u_1|^2+u_2|^2)^2.$$

Because of the assumption $Q^2=0$, p_μ is a null-vector and the transformation of Eq. (VIII.27) does not, of course, change this property of p_μ.

If the complex ket $|\chi\rangle$ satisfies Maxwell's equations [Eq. (III.4)], then it is easy to see that $|\psi_\nu\rangle$ will satisfy the two-component free neutrino equation

$$i\hbar(\partial/\partial t)|\psi_\nu\rangle=H|\psi_\nu\rangle, \qquad \text{(VIII.29)}$$

where

$$H=-i\hbar c\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}.$$

The equation $\nabla\cdot\boldsymbol{\chi}=0$ is transformed into

$$\langle\psi_\nu|\mathrm{f}(\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})|\psi_\nu\rangle=0, \qquad \text{(VIII.30)}$$

which includes the polarization states of the neutrino.

These results for one-particle theory imply that all three charge states satisfy the same neutrino equation and hence a chargeless neutrino is described by a complex wave function $|\psi_\nu\rangle$.

The equation for antineutrino[10] can be obtained in the same way by considering the projection of $|\chi^*\rangle$ on to the neutral plane $Q^*=0$ with the same projection operator. The resulting wave function because of the noninvariance under charge conjugation[11,12] is not the same as the complex conjugate of $|\psi_\nu\rangle$.

The possibility of using a complex wave function for the photon enables us to describe a neutrino in the same was as a neutral particle and also, instead of a Majorana neutrino, one obtains neutrino and antineutrino as different particles.

IX. CONCLUSION

In this paper only a sketch of the complex group is given. We feel that a more detailed and rigorous discussion of the complex representation is highly desirable. It is hoped that this representation of the Lorentz group will find some applications in elementary particle physics. In particular, the concept of electric charge seems to fit in best in the complex representation where antilinear operations play a basic role. For example, the possibility of having a charge coordinate, in addition to spin coordinate associated with a Dirac wave function and hence a simultaneous description of three charge states of fermions in terms of 12 component wave functions, seems to be quite feasible. Complex group may even enable us to obtain, in terms of appropriate projection operators involving γ_5, a simultaneous description of mass and massless fermion fields.[13] Furthermore, the charge and isotopic spin spaces may find a unified basis in the complex group.

It has always been accepted that only real wave functions should be used for the description of neutral mesons. In the light of experimental facts and theoretical possibilities offered by the complex representation, one feels that the use of a real wave function (for any field) is not a necessity. The latter possibility for neutral mesons has already been discussed.[14] Actually, the neutral state as one of the three states of charge is a complex component of a vector in charge space.

Complex group seems to have more scope for a possibility of discovering new quantum numbers and abstract symmetry operations. As long as a symmetry operation belongs to a certain representation of Lorentz group, its usefulness in elementary particle physics increases with its abstractness and strangeness.

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[10] The corresponding situation for the photon field can be described as a "charge conjugation" where particle and antiparticle properties are to be attributed to two different states of polarization.

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Asymptotic Properties of a Boson Field with Given Source*

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Some mathematical questions are answered in the theory of quantized boson fields with given linear source distribution. It is proved that the total Hamiltonian in the Fock representation is self-adjoint. Unitary operators governing the evolution of the system in the interaction picture are defined, and conditions given for their weak and strong convergence at remote times.

INTRODUCTION

THE theory of convergence to the Møller wave matrix, and to the S matrix, for wave packet scattering by classical potentials, has recently been put on a rigorous mathematical foundation.[1–9] It may now be of interest to begin similar study of a second-quantized case by discussing the simplest such, the solvable problem of bosons acted upon linearly by a given, extended, unquantized source.[10]

In theorem 1 we prove that the total Hamiltonian H_{total} is the closure of the essentially self-adjoint sum $H_{\text{free}}+H_{\text{interaction}}$ of the free-field and interaction Hamiltonians. Since H_{free} is already known to be self-adjoint, the functional calculus for such operators can now be used to define $U(t_2,t_1)=\exp(iH_{\text{free}}t_2)\times\exp[iH_{\text{total}}(t_1-t_2)]\exp(-iH_{\text{free}}t_1)$, the unitary which transforms the field at time t_1 into that at time t_2, in the interaction picture. In theorem 2 we prove that the weak limit as $t\to\pm\infty$ of $U(0,t)$ exists and is the scalar multiple of a unitary operator $U(0,\pm\infty)$, the Møller wave operator, with $H_{\text{total}}U(0,\pm\infty)=U(0,\pm\infty)H_{\text{free}}$. For time-dependent source, $U(t_2,t_1)$ will also be given an explicit definition, with sufficiency conditions for weak and strong convergence to the S operator $U(+\infty,-\infty)$ as $t_2\to+\infty$ and $t_1\to-\infty$.

Our proofs depend in an essential way on the fact that the external source is given, i.e., that its behavior has been prescribed in advance and does not depend on the field. Further, since the source appears linearly in H_{total} and point sources are excluded, the model is "solvable," H_{total} and H_{free} are unitarily equivalent. This equivalence is easy to see in the finite dimensional case where it is just a translation of origin to remove the linear term from a quadratic form. Unfortunately, much of the present paper must be devoted to a verification that this simple formal manipulation is actually valid in some infinite dimensional cases.

By our three restrictions on the source (given, linear, extended) we have withdrawn from the fundamental difficulties afflicting quantum field theory. As partial compensation, we are able to give a mathematically rigorous treatment of asymptotic properties of solutions of the dynamical equations, and hope thereby to attract into this strange field those mathematicians who have enjoyed proving quite similar theorems in the rather dissimilar subject of classical differential equations.

DEFINITIONS

Given the Hilbert space $\mathfrak{R}$ whose elements represent states of a single boson, we form the Fock[11] space

$$\mathfrak{F}=\sum_{n=0}^{\infty}\oplus\mathfrak{R}^{(n)},$$

where $\mathfrak{R}^{(n)}=\mathfrak{R}\otimes\cdots\otimes\mathfrak{R}$ is the tensor product of $\mathfrak{R}$ with itself n times. States of the boson field are represented by elements of the subspace

$$\mathfrak{S}=\sum_{n=0}^{\infty}\oplus\mathfrak{S}^{(n)}$$

of symmetric tensors in $\mathfrak{F}$. $\mathfrak{S}_0$ is defined to be the dense linear manifold of all

$$\sum_{n=0}^{\infty}\oplus f_n\in\mathfrak{S}$$

such that $f_n\neq0$ for only a finite number of n's. If T is any transformation of $\mathfrak{S}$, then T_0 will be its restriction to $\mathfrak{S}_0$. If H is a self-adjoint transformation on $\mathfrak{R}$, then

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[10] See Sec. 7 of G. Wentzel, *Einfuhrung in die Quantentheorie der Wellenfelder* (Franz Deuticke, Leipzig, Germany, 1943), for use of this approximation in the theory of neutral scalar mesons; also S. Tomonaga, Progr. Theoret. Phys. (Kyoto) **2**, 6 (1947); and L. van Hove, Physica **18**, 145 (1952). For electrodynamics: J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1955), Chaps. 14–15, and Chap. 16, Sec. 1, p. 397. For certain phonon problems: J. Bardeen, *Handbuch der Physik* (Springer-Verlag, Berlin, 1956), Vol. XV, Sec. 44, p. 365. A more mathematical treatment of given source distributions is contained in K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields* (Interscience Publishers, Inc., New York, 1953), Part III.
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$d\Gamma(H)$ is the closure of the densely defined linear transformation

$$\sum_{n=0}^{\infty}\oplus(H\otimes I^{(n-1)}+I\otimes H\otimes I^{(n-2)}+\cdots+I^{(n-1)}\otimes H)$$

on $\mathfrak{S}$.[12] For $\phi\in\mathfrak{R}$, $C(\phi)$ and $C^*(\phi)$ are the corresponding creation and annihilation operators,[12] and we define

$$p(\phi)=i[C(\phi)-C^*(\phi)]^\sim/\sqrt{2},$$
$$q(\phi)=[C(\phi)+C^*(\phi)]^\sim/\sqrt{2},$$

where $[\cdot]^\sim$ is the mapping which assigns to a closable operator its closure.[13]

For example, take the case of neutral scalar mesons of mass $m\geq 0$. Then $\mathfrak{R}$ will be all complex-valued square-integrable functions on a certain measure space, namely, the set of all real quadruples (k_0,k_1,k_2,k_3) such that $k_0^2-k_1^2-k_2^2-k_3^2=m^2$, $k_0\geq 0$ (positive-frequency hyperboloid in energy-momentum space), furnished with a measure invariant under the Lorentz group. $\mathfrak{S}^{(n)}$, the n-meson state space, can then be represented as all complex-valued symmetric functions of n such quadruples, square-integrable with respect to the product measure.

The group of unitary transformations on $\mathfrak{R}$ is represented in those on $\mathfrak{S}$ by

$$\Gamma: U\rightarrow\Gamma(U)=\sum_{n=0}^{\infty}\oplus U^{(n)},$$

where $U^{(n)}$, the tensor product of U with itself n times, operates on $\mathfrak{S}^{(n)}$. The differential $d\Gamma$ of this representation takes infinitesimal generators of one-parameter unitary groups on $\mathfrak{R}$ into such generators on $\mathfrak{S}$. In particular, it takes the single-meson Hamiltonian H, given by

$$(H\psi)(k_0,k_1,k_2,k_3)=k_0\psi(k_0,k_1,k_2,k_3)$$

for $\psi\in\mathfrak{R}$, into the free-field Hamiltonian $H_{\text{free}}=d\Gamma(H)$.

The letters p and q are used to express interaction between the field and an external system: either action of the field on the external system, as in measurement of the field value averaged over a test body represented by the test function ϕ, or action of the external system on the field, when to H_{free} must be added an $H_{\text{interaction}}$.

CANONICAL ISOMORPHISM

The dependence of $\mathfrak{S}$ on $\mathfrak{R}$ is exhibited explicitly in the notation

$$\mathfrak{S}(\mathfrak{R})=\sum_{n=0}^{\infty}\oplus\mathfrak{S}^{(n)}(\mathfrak{R}),$$

in order to make use of a canonical isomorphism

$$\mathfrak{S}(\mathfrak{M}_1\oplus\cdots\oplus\mathfrak{M}_m)\cong\mathfrak{S}(\mathfrak{M}_1)\otimes\cdots\otimes\mathfrak{S}(\mathfrak{M}_m),$$

of Segal.[14]

By the associativity of $\oplus$ and of $\otimes$, we need only define $\cong$ for $m=2$.

Let P_i, $i=1,2$, be the projection of $\mathfrak{M}_1\oplus\mathfrak{M}_2$ on $\mathfrak{M}_i$, and P_{n_1,n_2} the projection

$$P_{n_1,n_2}=\sum i_1+\cdots+i_{n(1)+n(2)}=n_1+2n_2 P_{i_1}\otimes\cdots\otimes P_{i_{n(1)+n(2)}}$$

in $\mathfrak{S}^{(n_1+n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$. Then

$$\mathfrak{S}(\mathfrak{M}_1\oplus\mathfrak{M}_2)=\sum_{n_1,n_2=0}^{\infty}\oplus P_{n_1,n_2}\mathfrak{S}^{(n_1+n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$$

because the $P_{i_1}\otimes\cdots\otimes P_{i_n}$ are a set of orthogonal projections such that

$$\sum_{n_1=0}^{n}P_{n_1,n-n_1}=\sum i_1,\cdots,i_n=1,2 P_{i_1}\otimes\cdots\otimes P_{i_n}$$
$$=(P_1+P_2)^{(n)}=I^{(n)}$$

on $(\mathfrak{M}_1\oplus\mathfrak{M}_2)^{(n)}$.

If $g_{n_1,n_2}\in P_{n_1,n_2}\mathfrak{S}^{(n_1+n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$, then

$$\|g_{n_1,n_2}\|^2=\|P_{n_1,n_2}g_{n_1,n_2}\|^2=\sum i_1+\cdots+i_{n(1)+n(2)}=n_1+2n_2$$
$$\times\|P_{i_1}\otimes\cdots\otimes P_{i_{n(1)+n(2)}}\cdot g_{n_1,n_2}\|^2.$$

The symmetry of g_{n_1,n_2} implies equality of all these summands, so

$$\|g_{n_1,n_2}\|^2=\frac{(n_1+n_2)!}{n_1!n_2!}\|P_1^{(n_1)}\otimes P_2^{(n_2)}g_{n_1,n_2}\|^2,$$

and the mapping

$$\sum_{n_1,n_2=0}^{\infty}\oplus g_{n_1,n_2}\rightarrow\sum_{n_1,n_2=0}^{\infty}\oplus\left[\frac{(n_1+n_2)!}{n_1!n_2!}\right]^{\frac{1}{2}}P_1^{(n_1)}\otimes P_2^{(n_2)}g_{n_1,n_2}$$

of $\mathfrak{S}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$ into

$$\sum_{n_1,n_2=0}^{\infty}\oplus(\mathfrak{M}_1^{(n_1)}\otimes\mathfrak{M}_2^{(n_2)})$$

is an isometry. The symmetry of g_{n_1,n_2} also implies that the mapping

$$g_{n_1,n_2}\rightarrow\left[\frac{(n_1+n_2)!}{n_1!n_2!}\right]^{\frac{1}{2}}P_1^{(n_1)}\otimes P_2^{(n_2)}g_{n_1,n_2}$$

of $P_{n_1,n_2}\mathfrak{S}^{(n_1+n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$ into $\mathfrak{M}_1^{(n_1)}\otimes\mathfrak{M}_2^{(n_2)}$ is actually onto $\mathfrak{S}^{(n_1)}(\mathfrak{M}_1)\otimes\mathfrak{S}^{(n_2)}(\mathfrak{M}_2)$, so we have an isomorphism

$$\mathfrak{S}(\mathfrak{M}_1\oplus\mathfrak{M}_2)\leftrightarrow\sum_{n_1,n_2=0}^{\infty}\oplus[\mathfrak{S}^{(n_1)}(\mathfrak{M}_1)\otimes\mathfrak{S}^{(n_2)}(\mathfrak{M}_2)].$$

[12] J. M. Cook, Trans. Am. Math. Soc. **74**, 222 (1953). [We replace Ω and ω of this reference by the more suggestive notation $d\Gamma$ and C of I. E. Segal, *ibid.* **81**, 106 (1956).]

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[14] *Les Problemes Mathématiques de la Théorie Quantique des Champs* (Centre National de la Recherche Scientifique, Paris, 1959), p. 69, note 3.

This is followed by the natural isomorphism

$$\sum_{n_1,n_2=0}^{\infty}\oplus[\mathfrak{S}^{(n_1)}(\mathfrak{M}_1)\otimes\mathfrak{S}^{(n_2)}(\mathfrak{M}_2)]\leftrightarrow$$

$$[\sum_{n_1=0}^{\infty}\oplus\mathfrak{S}^{(n_1)}(\mathfrak{M}_1)]\otimes[\sum_{n_2=0}^{\infty}\oplus\mathfrak{S}^{(n_2)}(\mathfrak{M}_2)]$$

given by the distributivity of $\otimes$ with respect to $\oplus$; and the definition of $\cong$ is complete.

In Segal's formulation this isomorphism is expressed as an infinite dimensional generalization of the familiar relation $\mathfrak{L}_2(\mathfrak{M}_1\oplus\mathfrak{M}_2)\cong\mathfrak{L}_2(\mathfrak{M}_1)\otimes L_2(\mathfrak{M}_2)$ for Hilbert spaces of square-integrable functions over the finite dimensional vector spaces $\mathfrak{M}_1$, $\mathfrak{M}_2$, and $\mathfrak{M}_1\oplus\mathfrak{M}_2$.

We will use $\cong$ to reduce assertions about $\mathfrak{S}(\mathfrak{R})$ to more easily proven assertions involving subspaces of $\mathfrak{R}$.

DIAGONALIZATION OF THE TOTAL HAMILTONIAN

In theorem 1 a unitary operator will be constructed which transforms the total into the free-field Hamiltonian. The latter is self-adjoint with known spectrum (if true of the single-particle Hamiltonian from which it was constructed), so this solves the diagonalization problem. First step in the proof is "completion of the square" for single-particle Hamiltonians on one-dimensional spaces.

Five preliminary lemmas must be proved which state, roughly:

(1) If the H_{total}'s for each of a finite number of different Fock spaces are self-adjoint, then so is H_{total} for Fock space over the direct sum of the corresponding single-particle spaces.

(2) H_{total} is self-adjoint, if the single-particle Hamiltonian is bounded away from zero.

(3) H_{total} is unitarily equivalent to H_{free} if it is approximated by operators with a similar property.

(4) Translation of the origin of single-particle space causes a unitary transformation of Fock space which induces the expected canonical transformation of the q's.

(5) When acted upon by such a unitary transformation, the bare source becomes "clothed," the particle number having a Poisson distribution.

Lemma 1. Let $[\{d\Gamma(H_i)+q(\phi)\}_0]^\sim$ be self-adjoint on $\mathfrak{S}(\mathfrak{M}_i)$; $i=1,\cdots,m$; $\phi_i\in\mathfrak{M}_i$. Then

$$[\{d\Gamma(H_1\oplus\cdots\oplus H_m)+q(\phi_1\oplus\cdots\oplus\phi_m)\}_0]^\sim$$

is self-adjoint on $\mathfrak{S}(\mathfrak{M}_1\oplus\cdots\oplus\mathfrak{M}_m)$.

Proof.

By associativity, we may assume $m=2$.

In $\mathfrak{S}^{(n_1+n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$ we have

$$P_1^{(n_1)}\otimes P_2^{(n_2)}[I^{(k-1)}\otimes(H_1\oplus 0)\otimes I^{(n_1+n_2-k)}]$$
$$=P_1^{(k-1)}\otimes(H_1\oplus 0)\otimes P_1^{(n_1-k)}\otimes P_2^{(n_2)}\quad\text{if}\quad 1\le k\le n,$$
$$\subseteq 0^{(n_1+n_2)}\ \text{otherwise.}$$

So

$$\Big(\sum_{n_1,n_2=0}^{\infty}\oplus\Big\{\Big[\frac{(n_1+n_2)!}{n_1!n_2!}\Big]^{\frac{1}{2}}P_1^{(n_1)}\otimes P_2^{(n_2)}\Big\}\Big)d\Gamma(H_1\oplus 0)_0$$
$$\subseteq\Big(\sum_{n_1,n_2=0}^{\infty}\oplus\{[\sum_{k=1}^{n_1}P_1^{(k-1)}\otimes(H_1\oplus 0)\otimes P_1^{(n_1-k)}]^\sim$$
$$\otimes P_2^{(n_2)}\}\Big[\frac{(n_1+n_2)!}{n_1!n_2!}\Big]^{\frac{1}{2}}P_1^{(n_1)}\otimes P_2^{(n_2)}\Big)_0$$

and, under the isomorphism

$$\mathfrak{S}(\mathfrak{M}_1\oplus\mathfrak{M}_2)\cong\mathfrak{S}(\mathfrak{M}_1)\otimes\mathfrak{S}(\mathfrak{M}_2)$$

given on $P_{n_1,n_2}\mathfrak{S}^{(n_1+n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$ by

$$g_{n_1,n_2}\leftrightarrow\Big[\frac{(n_1+n_2)!}{n_1!n_2!}\Big]^{\frac{1}{2}}P_1^{(n_1)}\otimes P_2^{(n_2)}g_{n_1,n_2},$$

we have $d\Gamma(H_1\oplus 0)_o\cong[d\Gamma(H_1)\otimes I_2]_o$, where the subscript o applied to an operator on $\mathfrak{S}(\mathfrak{M}_1)\otimes\mathfrak{S}(\mathfrak{M}_2)$ means its restriction to the set of all

$$\sum_{n_1,n_2=0}^{\infty}\oplus f_{n_1,n_2}$$

such that $f_{n_1,n_2}\neq 0$ for only a finite number of n_1, n_2; i.e., its restriction to $[\mathfrak{S}(\mathfrak{M}_1)\otimes(\mathfrak{M}_2)]_o\cong\mathfrak{S}_0(\mathfrak{M}_1\oplus\mathfrak{M}_2)$.

Similarly, $d\Gamma(0\oplus H_2)_o\cong[I_1\otimes d\Gamma(H_2)]_o$.

The behavior of $q(\phi_1\oplus 0)_o$ under the canonical isomorphism $\mathfrak{S}(\mathfrak{M}_1\oplus\mathfrak{M}_2)\cong\mathfrak{S}(\mathfrak{M}_1)\otimes\mathfrak{S}(\mathfrak{M}_2)$ is determined by that of $C^*(\phi_1\oplus 0)$, which maps

$$P_{n_1,n_2}\mathfrak{S}^{(n_1+n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$$

into

$$P_{n_1-1,n_2}\mathfrak{S}^{(n_1-1,n_2)}(\mathfrak{M}_1\oplus\mathfrak{M}_2)$$

by

$$g_{n_1,n_2}\to(n_1+n_2)^{\frac{1}{2}}[(\phi_1\oplus 0)\otimes]^*g_{n_1,n_2},$$

where $[(\phi_1\oplus 0)\otimes]^*$ is the bounded linear transformation uniquely defined by its action

$$[(\phi_1\oplus 0)\otimes]^*\psi_1\otimes\cdots\otimes\psi_{n_1+n_2}$$
$$=(\psi_1,(\phi_1\oplus 0))\psi_2\otimes\cdots\otimes\psi_{n_1+n_2}$$

on decomposable tensors.[15] Therefore,

$$\Big[\frac{(n_1-1+n_2)!}{(n_1-1)!n_2!}\Big]^{\frac{1}{2}}P_1^{(n_1-1)}\otimes P_2^{(n_2)}C^*(\phi_1\oplus 0)g_{n_1,n_2}$$
$$=\Big[\frac{(n_1+n_2)!}{(n_1-1)!n_2!}\Big]^{\frac{1}{2}}P_1^{(n_1-1)}\otimes P_2^{(n_2)}[(\phi_1\oplus 0)\otimes]^*g_{n_1,n_2}$$
$$=[(\phi_1\oplus 0)\otimes]^*\Big[\frac{(n_1+n_2)!}{(n_1-1)!n_2!}\Big]^{\frac{1}{2}}P_1^{(n_1)}\otimes P_2^{(n_2)}g_{n_1,n_2}$$
$$\text{(since } P_1\cdot\phi_1\oplus 0=\phi_1\oplus 0)$$
$$=n_1^{\frac{1}{2}}[(\phi_1\oplus 0)\otimes]^*\Big\{\Big[\frac{(n_1+n_2)!}{n_1!n_2!}\Big]^{\frac{1}{2}}P_1^{(n_1)}\otimes P_2^{(n_2)}g_{n_1,n_2}\Big\}.$$

In other words, $C^*(\phi_1\oplus 0)_o\cong[C^*(\phi_1)\otimes I_2]_o$.

[15] See footnote 11, p. 637; also, see footnote 12, Sec. 4, pp. 228–9.

The isomorphism is adjoint preserving, so $C(\phi_1\oplus 0)_o \cong [C(\phi_1)\otimes I_2]_o$ also.

Therefore $q(\phi_1\oplus 0)_o \cong [q(\phi_1)\otimes I_2]_o$.

Similarly $q(0\oplus\phi_2)_o \cong [I_1\otimes q(\phi_2)]_o$.

So

$$\begin{aligned}&[d\Gamma(H_1\oplus H_2)+q(\phi_1\oplus\phi_2)]_o\\&=d\Gamma(H_1\oplus H_2)_o+q(\phi_1\oplus\phi_2)_o\\&=d\Gamma(H_1\oplus 0)_o+q(\phi_1\oplus 0)_o+d\Gamma(0\oplus H_2)_o+q(0\oplus\phi_2)_o\\&\cong[d\Gamma(H_1)\otimes I_2]_o+[q(\phi_1)\otimes I_2]_o\\&\quad+[I_1\otimes d\Gamma(H_2)]_o+[I_1\otimes q(\phi_2)]_o\\&=([\{d\Gamma(H_1)+q(\phi_1)\}_0]^\sim\otimes I_2)_o\\&\qquad+(I_1\otimes[\{d\Gamma(H_2)+q(\phi_2)\}_0]^\sim)_o.\end{aligned}$$

Let

$$B_i=[\{d\Gamma(H_i)+q(\phi_i)\}_o]^\sim.$$

By hypothesis, B_i is a self-adjoint operator on $\mathfrak{S}(\mathfrak{M}_i)$. We must show that the closure of $(B_i\otimes I_2)_o+(I_1\otimes B_2)_o$ exists and is self-adjoint.

Existence of the closure follows from the fact that $(B_i\otimes I_2)_o+(I_1\otimes B_2)_o$ is symmetric, i.e., is contained in its adjoint, a closed operator. To prove the closure self-adjoint, we first show

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim\supseteq(B_1\otimes I_2+I_1\otimes B_2)^\sim.$$

Let $f_i\in\mathfrak{D}B_i$. By hypothesis, there exist $f_{i,n}\in\mathfrak{S}(\mathfrak{M}_i)_o$ such that $f_{i,n}\to f_i$ and $B_if_{i,n}\to B_if_i$, i.e., such that $f_{1,n}\otimes f_{2,n}\to f_1\otimes f_2$ and

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o](f_{1,n}\otimes f_{2,n})\to(B_1f_1)\otimes f_2+f_1\otimes(B_2f_2).$$

Therefore $f_1\otimes f_2\in\mathfrak{D}[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim$ and

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim(f_1\otimes f_2)=(B_1f_1)\otimes f_2+f_1\otimes(B_2f_2).$$

Now let $B_i=\int\lambda dE_{i,\lambda}$, and

$$g_\Delta\in[(E_{1,\Delta}-E_{1,-\Delta})\otimes(E_{2,\Delta}-E_{2,-\Delta})]\mathfrak{S}(\mathfrak{M}_1)\otimes\mathfrak{S}(\mathfrak{M}_2).$$

If

$$\{g_{i,k}\}_{k=1}^{\infty}$$

is a complete orthonormal set in $(E_{i,\Delta}-E_{i,-\Delta})\mathfrak{S}(\mathfrak{M}_i)$, then

$$g_{\Delta,n}=\sum_{k_1,k_2=1}^{n}(g_\Delta,g_{1,k_1}\otimes g_{2,k_2})g_{1,k_1}\otimes g_{2,k_2}\to g_\Delta \text{ as } n\to\infty,$$

and [since $g_{i,k}\in\mathfrak{D}B_i$ and $B_1\otimes I_2+I_1\otimes B_2$ is bounded on $(E_{1,\Delta}-E_{1,-\Delta})\otimes(E_{2,\Delta}-E_{2,-\Delta})\cdot\mathfrak{S}(\mathfrak{M}_1)\otimes\mathfrak{S}(\mathfrak{M}_2)$] we have

$$\begin{aligned}&[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim g_{\Delta,n}\\&\quad=(B_1\otimes I_2+I_1\otimes B_2)g_{\Delta,n}\to(B_1\otimes I_2+I_1\otimes B_2)g_\Delta.\end{aligned}$$

In other words, $g_\Delta\in\mathfrak{D}[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim$ and

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim g_\Delta=(B_1\otimes I_2+I_1\otimes B_2)g_\Delta.$$

Finally, let $g\in\mathfrak{D}[B_1\otimes I_2+I_1\otimes B_2]^\sim$ and

$$g_\Delta=(E_{1,\Delta}-E_{1,-\Delta})\otimes(E_{2,\Delta}-E_{2,-\Delta})g.$$

Then, by the preceding paragraph,

$$g_\Delta\in\mathfrak{D}[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim$$

and

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim g_\Delta=(B_1\otimes I_2+I_1\otimes B_2)g_\Delta.$$

$E_{1,\lambda_1}\otimes E_{2,\lambda_2}$ is a two-parameter spectral decomposition,[16] so $[B_1\otimes I_2+I_1\otimes B_2]^\sim$ is self-adjoint. Further, $g_\Delta\to g$ and

$$(B_1\otimes I_2+I_1\otimes B_2)g_\Delta\to[B_1\otimes I_2+I_1\otimes B_2]^\sim g.$$

Therefore $g\in\mathfrak{D}[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim$ and

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim g=[B_1\otimes I_2+I_1\otimes B_2]^\sim g;$$

in other words,

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim\supseteq[B_1\otimes I_2+I_1\otimes B_2]^\sim.$$

But $[B_1\otimes I_2+I_1\otimes B_2]^\sim$ is maximal (since self-adjoint)[17] so

$$[(B_1\otimes I_2)_o+(I_1\otimes B_2)_o]^\sim=[B_1\otimes I_2+I_1\otimes B_2]^\sim.$$

Corollary.

$$\begin{aligned}&[\{d\Gamma(H_1\oplus H_2)+q(\phi_1\oplus\phi_2)\}_o]^\sim\\&\quad\cong[[[\{(d\Gamma(H_1)+q(\phi_1)\}_o]^\sim\otimes I_2\\&\qquad+I_1\otimes[\{d\Gamma(H_2)+q(\phi_2)\}_o]^\sim]^\sim\end{aligned}$$

if $[\{d\Gamma(H_1\oplus H_2)+q(\phi_1\oplus\phi_2)\}_o]^\sim$ is self-adjoint.

Proof.

$$\begin{aligned}&[d\Gamma(H_1\oplus H_2)+q(\phi_1\oplus\phi_2)]_o\\&=d\Gamma(H_1\oplus 0)_o+q(\phi_1\oplus 0)_o+d\Gamma(0\oplus H_2)_o+q(0\oplus\phi_2)_o\\&\cong[d\Gamma(H_1)\otimes I_2]_o+[q(\phi_1)\otimes I_2]_o\\&\quad+[I_1\otimes d\Gamma(H_2)]_o+[I_1\otimes q(\phi_2)]_o\\&=\{[d\Gamma(H_1)+q(\phi_1)]\otimes I_2\}_o+\{I_1\otimes[d\Gamma(H_2)+q(\phi_2)]\}_o\end{aligned}$$

as before.

Therefore,

$$\begin{aligned}&[\{d\Gamma(H_1\oplus H_2)+q(\phi_1\oplus\phi_2)\}_o]^\sim\\&\cong[\{[d\Gamma(H_1)+q(\phi_1)]\otimes I_2\}_o\\&\quad+\{I_1\otimes[d\Gamma(H_2)+q(\phi_2)]\}_o]^\sim\subseteq[\{[d\Gamma(H_1)\\&\quad+q(\phi_1)]_o\otimes I_2+I_1\otimes[d\Gamma(H_2)+q(\phi_2)]_o\}]^\sim\\&\subseteq[[[\{d\Gamma(H_1)+q(\phi_1)\}_o]^\sim\otimes I_2\\&\qquad+I_1\otimes[\{d\Gamma(H_2)+q(\phi_2)\}_o]^\sim]^\sim.\end{aligned}$$

But $[\{d\Gamma(H_1\oplus H_2)+q(\phi_1\oplus\phi_2)\}_o]^\sim$ is maximal because self-adjoint by hypothesis.

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[16] B. V. Nagy, *Spektraldarstellung Linearer Transformationen des Hilbertschen Raumes* (Springer-Verlag, Berlin, 1942), p. 46.

[17] See footnote 16, Chap. V, Sec. 4, p. 33; or footnote 13, p. 50, Th. 2.13.

Lemma 2. If H is self-adjoint and $\geq I$, then

$$[\{d\Gamma(H)+q(\phi)\}_o]^\sim$$

is also self-adjoint.

Proof.

First we assume $H\geq 3\|\phi\|I$.

To prove $[d\Gamma(H)+C(\phi)+C^*(\phi)]_o$ essentially self-adjoint under these conditions, we need prove that its deficiency indices are zero, i.e., that if

$$g=\sum_{n=0}^{\infty}\oplus g_n\in\mathfrak{S}$$

is orthogonal to

$$[d\Gamma(H)+C(\phi)+C^*(\phi)\pm iI]\mathfrak{D}d\Gamma(H)+C(\phi)+C^*(\phi),$$

then $g=0$.[18] So, let

$$0=(g,[d\Gamma(H)+C(\phi)+C^*(\phi)\pm iI]f_n)$$

for $f_n\in\mathfrak{D}d\Gamma(H)\bigcap\mathfrak{S}^{(n)}$. Then

$$\begin{aligned}0&=(g_{n-1}\oplus g_n\oplus g_{n+1},[d\Gamma(H)+C(\phi)+C^*(\phi)\pm iI]f_n)\\&=(g_n,[d\Gamma(H)\pm iI]f_n)+(C(\phi)g_{n-1}+C^*(\phi)g_{n+1},f_n).\end{aligned}$$

Therefore $g_n\in\mathfrak{D}[d\Gamma(H)\pm iI]^*$ and, since the self-adjointness of $d\Gamma(H)$ implies

$$[d\Gamma(H)\pm iI]^*=d\Gamma(H)\mp iI,$$

we have

$$[d\Gamma(H)\mp iI]g_n=-C(\phi)g_{n-1}-C^*(\phi)g_{n+1}$$

if $n=1, 2, \cdots$; $\mp ig_0=-(g_1,\phi)$. Therefore

$$\|[d\Gamma(H)\mp iI]g_n\|\leq\|C(\phi)g_{n-1}\|+\|C^*(\phi)g_{n+1}\|,\qquad n=1, 2, \cdots$$

and

$$\|g_0\|\leq\|g_1\|\cdot\|\phi\|.$$

But

$$\|[d\Gamma(H)\mp iI]g_n\|\geq\|d\Gamma(H)g_n\|.$$

Further, $H\geq 3\|\phi\|I$ implies $d\Gamma(H)\geq 3\|\phi\|d\Gamma(I)$,[19] so

$$\|d\Gamma(H)g_n\|\geq 3\|\phi\|\cdot\|d\Gamma(I)g_n\|=3n\|\phi\|\cdot\|g_n\|.$$

So

$$\|[d\Gamma(H)\mp iI]g_n\|\geq 3n\|\phi\|\cdot\|g_n\|,$$

and

$$3n\|\phi\|\cdot\|g_n\|\leq\|C(\phi)g_{n-1}\|+\|C^*(\phi)g_{n+1}\|,\quad n=1, 2, \cdots.$$

From the polar decomposition of $C(\phi)$ and $C^*(\phi)$, it can be seen[20] that

$$\|C(\phi)g_{n-1}\|\leq n^{\frac{1}{2}}\|\phi\|\cdot\|g_{n-1}\|$$

and

$$\|C^*(\phi)g_{n+1}\|\leq(n+1)^{\frac{1}{2}}\|\phi\|\cdot\|g_{n+1}\|.$$

If $\phi=0$, the lemma is obvious,[21] so we can assume $\|\phi\|\neq 0$. Then $3n\|g_n\|\leq n^{\frac{1}{2}}\|g_{n-1}\|+(n+1)^{\frac{1}{2}}\|g_{n+1}\|$, i.e., $(n+1)^{\frac{1}{2}}\|g_{n+1}\|\geq 3n\|g_n\|-n^{\frac{1}{2}}\|g_{n-1}\|$ for $n=1, 2, \cdots$.

By the real homogeneity of $d\Gamma$, C, and C^*, we may assume $\|\phi\|=1$. Then $\|g_0\|\leq\|g_1\|\cdot\|\phi\|$ implies $\|g_1\|\geq\|g_0\|$.

If $n\geq 1$, then $\|g_{n+1}\|\geq(3n\cdot\|g_n\|-n^{\frac{1}{2}}\|g_{n-1}\|)(n+1)^{-\frac{1}{2}}$ and $(3n-n^{\frac{1}{2}})(n+1)^{-\frac{1}{2}}\geq 1$, so $\|g_n\|\geq\|g_{n-1}\|$ implies

$$\|g_{n+1}\|\geq(3n-n^{\frac{1}{2}})(n+1)^{-\frac{1}{2}}\|g_n\|\geq\|g_n\|.$$

We already know $\|g_1\|\geq\|g_0\|$, so by induction we conclude $\|g_0\|\leq\|g_1\|\leq\|g_2\|\leq\|g_3\|\leq\cdots$ etc. Therefore

$$\sum_{n=0}^{\infty}\|g_n\|^2=\|g\|^2<\infty$$

only when $g=0$, both defect indices of $[d\Gamma(H)+C(\phi)+C^*(\phi)]_o$ are zero, and the operator is essentially self-adjoint.

Now we want to remove the restriction $H\geq 3\|\phi\|I$ on $\|\phi\|$, so let $H\geq I$, and $\|\phi\|$ arbitrary.

Pick the integer m so large that $3m^{-\frac{1}{2}}\|\phi\|<1$, and let $\mathfrak{V}_m$ be the m-dimensional complex Hilbert space of all m tuples $(x_1,\cdots,x_m)$. Now, instead of H on $\mathfrak{R}$, consider $H\otimes I$ on $\mathfrak{R}\otimes\mathfrak{V}_m$; and instead of $\phi\in\mathfrak{R}$, consider $\phi\otimes v\in\mathfrak{R}\otimes\mathfrak{V}_m$, where $v=m^{-\frac{1}{2}}(1,1,\cdots,1)\in\mathfrak{V}_m$. Then $\mathfrak{R}\otimes\mathfrak{V}_m=\mathfrak{M}_1\oplus\cdots\oplus\mathfrak{M}_m$, where $\mathfrak{M}_i=\mathfrak{R}\otimes(\delta_1{}^i,\cdots,\delta_m{}^i)$; and $\phi\otimes v=\phi_1\oplus\cdots\oplus\phi_m$ with $\phi_i=m^{-\frac{1}{2}}\phi\otimes(\delta_1{}^i,\cdots,\delta_m{}^i)\in\mathfrak{M}_i$. The $\mathfrak{M}_i$ decompose $H\otimes I$ into $H\otimes I=H_1\oplus\cdots\oplus H_m$. Since $H_i\geq I_i>3m^{-\frac{1}{2}}\|\phi\|\cdot I_i=3\|\phi_i\|\cdot I_i$ in each $\mathfrak{M}_i$, the first part of the proof of this lemma shows that $[\{d\Gamma(H_i)+C(\phi_i)+C^*(\phi_i)\}_o]^\sim$ is self-adjoint on $\mathfrak{S}(\mathfrak{M}_i)$; and so, by lemma 1, and the real homogeneity of $d\Gamma$, C, and C^*, we can assert that

$$[\{d\Gamma(H\otimes I)+q(\phi\otimes v)\}_o]^\sim$$

is self-adjoint on $\mathfrak{S}(\mathfrak{R}\otimes\mathfrak{V}_m)$.

Now decompose $\mathfrak{V}_m$ differently: $\mathfrak{V}_m=\{v\}\oplus\{v\}^\perp$. By the corollary to lemma 1,

$$\begin{aligned}&[\{d\Gamma(H\otimes I)+q(\phi\otimes v)\}_o]^\sim\\&\quad\cong[[\{d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v)\}_o]^\sim\otimes I''\\&\qquad+I'\otimes[\{d\Gamma(H\otimes P_{\{v\}^\perp})+q(0)\}_o]^\sim]^\sim,\end{aligned}$$

where I' is the identity on $\mathfrak{S}(\mathfrak{R}\otimes\{v\})$ and I'' that on $\mathfrak{S}(\mathfrak{R}\otimes\{v\}^\perp)$.

Therefore

$$\begin{aligned}&[[\{d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v\}_o]^\sim\otimes I''\\&\qquad+I'\otimes[\{d\Gamma(H\otimes P_{\{v\}^\perp})+q(0)\}_o]^\sim]^\sim,\end{aligned}$$

in other words,

$$\begin{aligned}&[[\{d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v)\}_o]^\sim\otimes I''\\&\qquad+I'\otimes d\Gamma(H\otimes P_{\{v\}^\perp})]^\sim,\end{aligned}$$

is self-adjoint on $\mathfrak{S}(\mathfrak{R}\otimes\{v\})\otimes\mathfrak{S}(\mathfrak{R}\otimes\{v\}^\perp)$.

It commutes with $I'\otimes\exp[itd\Gamma(I\otimes P_{\{v\}^\perp})]$ because the latter, as an isomorphism, commutes with the invariantly defined operation $(\cdot)^\sim$ and then with the

[18] See footnote 16, p. 38; or footnote 13, p. 339.
[19] Footnote 12, p. 224, Cor. 2.
[20] Footnote 12, p. 229.
[21] Footnote 12, p. 223, Th. 1.

two summands. The first because

$$I'\otimes\exp[itd\Gamma(I\otimes P_{\{v\}^\perp})]$$

is an identity on $\mathfrak{S}(\mathfrak{R}\otimes\{v\})$, and the second because

$$\begin{aligned}&\exp[itd\Gamma(I\otimes P_{\{v\}^\perp})]\cdot d\Gamma(H\otimes P_{\{v\}^\perp})\\ &\qquad\times\exp[-itd\Gamma(I\otimes P_{\{v\}^\perp})]\\ &=d\Gamma[\exp(itI\otimes P_{\{v\}^\perp})\cdot H\otimes P_{\{v\}^\perp}\cdot\exp(-itI\otimes P_{\{v\}^\perp})]^{22}\\ &=d\Gamma\{[\exp(it)\cdot H\cdot\exp(-it)]\otimes P_{\{v\}^\perp}\}\\ &\qquad\text{(by the idempotence of } P_{\{v\}^\perp})\\ &=d\Gamma(H\otimes P_{\{v\}^\perp}).\end{aligned}$$

Since the self-adjoint operator

$$[[\{d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v)\}_o]^\sim\otimes I''+I'\otimes d\Gamma(H\otimes P_{\{v\}^\perp})]^\sim$$

commutes with every element of the one-parameter group $I'\otimes\exp[itd\Gamma(I\otimes P_{\{v\}^\perp})]$, it must commute with the projections in the spectral decomposition of the infinitesimal generator $I'\otimes d\Gamma(I\otimes P_{\{v\}^\perp})$.[23]

Zero is an eigenvalue in the point spectrum of $d\Gamma(I\otimes P_{\{v\}^\perp})$, with the corresponding eigenspace $\mathfrak{S}^{(0)}(\mathfrak{R}\otimes\{v\}^\perp)$; so

$$[[\{d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v)\}_o]^\sim\otimes I''+I'\otimes d\Gamma(H\otimes P_{\{v\}^\perp})]^\sim$$

is reduced by, and is self-adjoint in, the subspace $\mathfrak{S}(\mathfrak{R}\otimes\{v\})\otimes\mathfrak{S}^{(0)}(\mathfrak{R}\otimes\{v\}^\perp)$. But here $I'\otimes d\Gamma(H\otimes P_{\{v\}^\perp})$ is zero, so we have shown that

$$[[\{d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v)\}_o]^\sim\otimes I'']^\sim$$

is self-adjoint on $\mathfrak{S}(\mathfrak{R}\otimes\{v\})\otimes\mathfrak{S}^{(0)}(\mathfrak{R}\otimes\{v\}^\perp)$. Further, since $\mathfrak{S}^{(0)}(\mathfrak{R}\otimes\{v\}^\perp)$ is one-dimensional, we have also shown that $[\{d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v)\}_o]^\sim$ is self-adjoint on $\mathfrak{S}(\mathfrak{R}\otimes\{v\})$.

Finally, since $\{v\}$ is one-dimensional, $\mathfrak{R}\otimes\{v\}$ is isomorphic to $\mathfrak{R}$ in such a way that

$$H\otimes P_{\{v\}}\leftrightarrow H,\quad \phi\otimes v\leftrightarrow\phi,\quad \mathfrak{S}(\mathfrak{R}\otimes\{v\})\leftrightarrow\mathfrak{S}(\mathfrak{R}),$$

and

$$d\Gamma(H\otimes P_{\{v\}})+q(\phi\otimes v)\leftrightarrow d\Gamma(H)+q(\phi).$$

Lemma 3. Let H_k be a sequence of commuting, nonnegative self-adjoint operators such that $\phi\in\mathfrak{D}H_k$ and

$$[d\Gamma(H_k)+q(H_k\phi)+\tfrac{1}{2}(H_k\phi,\phi)]^\sim=e^{ip(\phi)}d\Gamma(H_k)e^{-ip(\phi)}.$$

If H is a self-adjoint operator, commuting with all H_k, such that

$$\phi\in\mathfrak{D}H,\ [d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]_o$$

is essentially self-adjoint, and $H_k\uparrow H$ strongly on $\mathfrak{D}H$; then

$$[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim=e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}.$$

[22] Footnote 12, p. 225, Th. 3.

[23] Footnote 16, p. 69.

Proof.

$H_k\uparrow H$ strongly on $\mathfrak{D}H$ implies $d\Gamma(H_k)\uparrow d\Gamma(H)$ strongly on $\mathfrak{D}d\Gamma(H)$. Therefore,

$$[d\Gamma(H_k)+q(H_k\phi)+\tfrac{1}{2}(H_k\phi,\phi)]^\sim\uparrow e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}$$

strongly on $\mathfrak{D}e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}$.

Let

$$f\in\mathfrak{D}[d\Gamma(H)+q(H\phi)+(H\phi,\phi)^{\frac{1}{2}}]_o.$$

Then $f\in\mathfrak{D}d\Gamma(H_k)\bigcap\mathfrak{D}q(H_k\phi)$ for all k [since $0\leq H_k\leq H$ implies $0\leq d\Gamma(H_k)\leq d\Gamma(H)$ and, therefore, $\mathfrak{D}d\Gamma(H_k)\supset\mathfrak{D}d\Gamma(H)$; also $\mathfrak{S}_0\subset\mathfrak{D}q(H_k\phi)$], and

$$\begin{aligned}&[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]f\\ &\qquad-[d\Gamma(H_k)+q(H_k\phi)+\tfrac{1}{2}(H_k\phi,\phi)]f\\ &\quad=d\Gamma(H-H_k)f+q[(H-H_k)\phi]f\\ &\qquad+\tfrac{1}{2}((H-H_k)\phi,\phi)f\to 0\quad\text{as}\quad k\to\infty.\end{aligned}$$

Since

$$f\in\mathfrak{D}e^{ip(\phi)}d\Gamma(H_k)e^{-ip(\phi)}\{=\mathfrak{D}[d\Gamma(H_k)+q(H_k\phi)+(H_k\phi,\phi)^{\frac{1}{2}}]^\sim\text{ by hypothesis}\}$$

and $\lim_{k\to\infty}e^{ip(\phi)}d\Gamma(H_k)e^{-ip(\phi)}f$ exists (by the previous sentence), we must have $f\in\mathfrak{D}e^{ip(\phi)}\cdot d\Gamma(H)e^{-ip(\phi)}$ and

$$\lim_{k\to\infty}e^{ip(\phi)}d\Gamma(H_k)e^{-ip(\phi)}f=e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}f$$

[by Lebesgue's bounded convergence theorem applied to the monotone increasing sequence of integrands in the simultaneous spectral decompositions of all $e^{ip(\phi)}d\Gamma(H_k)e^{-ip(\phi)}$ and $e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}$]. The limit has already been shown to equal $[d\Gamma(H)+q(H\phi)+\frac{1}{2}(H\phi,\phi)]_of$, so we conclude

$$e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}\supseteq[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]_o.$$

Therefore,

$$e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}\supseteq[\{d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)\}_o]^\sim.$$

But $[\{d\Gamma(H)+q(H\phi)+\frac{1}{2}(H\phi,\phi)\}_o]^\sim$ is self-adjoint by hypothesis, and, therefore, maximal, so

$$e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}=[\{d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)\}_o]^\sim.$$

Further,

$$d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)\supseteq[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]_o$$

implies

$$[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim\supseteq[\{d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)\}_o]^\sim$$

[existence of the closure of $d\Gamma(H)+q(H\phi)+\frac{1}{2}(H\phi,\phi)$ is guaranteed by its symmetricity[24]], and again the maximality of $[\{d\Gamma(H)+q(H\phi)+\frac{1}{2}(H\phi,\phi)\}_o]^\sim$ implies

$$[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim=[\{d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)\}_o]^\sim.$$

Lemma 4. $e^{+ip(\phi)}q(\phi_1)e^{-ip(\phi)}=q(\phi_1)+\mathrm{Re}(\phi,\phi_1)$.

[24] Footnote 16, p. 34.

Proof.

Let $f\in\mathfrak{S}_0$. Then, since $[q(\phi_1),p(\phi)]^{\sim}=i\,\mathrm{Re}(\phi,\phi_1)$,[25]

$$[q(\phi_1)ip(\phi)+\mathrm{Re}(\phi,\phi_1)]f=ip(\phi)q(\phi_1)f.$$

By induction (possible because all operators involved carry $\mathfrak{S}_0$ into itself)

$$[ip(\phi)]^n q(\phi_1)f=q(\phi_1)[ip(\phi)]^n f+n[ip(\phi)]^{n-1}\,\mathrm{Re}(\phi,\phi_1)f,$$

and, therefore,

$$\sum_{n=0}^{m}\frac{[ip(\phi)]^n}{n!}q(\phi_1)f=q(\phi_1)\sum_{n=0}^{m}\frac{[ip(\phi)]^n}{n!}f+\sum_{n=0}^{m-1}\frac{[ip(\phi)]^n}{n!}\times\mathrm{Re}(\phi,\phi_1)f.$$

As $m\to\infty$, the series

$$\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}f\quad\text{and}\quad\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}q(\phi_1)f$$

converge absolutely. [If g is in the subspace corresponding to

$$\sum_{k=0}^{l}\oplus\mathfrak{S}^{(k)},$$

then $ip(\phi)g$ is in that corresponding to

$$\sum_{k=0}^{l+1}\oplus\mathfrak{S}^{(k)},$$

and

$$\|ip(\phi)g\|\leq\|\phi\|\sqrt{2}(l+1)^{\frac{1}{2}}\|g\|$$

by the polar decompositions[26] of $C(\phi)$ and $C^*(\phi)$. Now apply the ratio test.]

Since $q(\phi_1)$ is closed, this means that

$$\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}f\in\mathfrak{D}q(\phi_1)$$

and

$$\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}q(\phi_1)f=q(\phi_1)\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}f+\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}\times\mathrm{Re}(\phi,\phi_1)f.$$

Further, whenever

$$\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}g$$

converges strongly, it must equal $e^{ip(\phi)}g$. [Let $p(\phi)=\int\lambda dE_\lambda$. Then

$$(E_\Lambda-E_{-\Lambda})\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}g=\sum_{n=0}^{\infty}(E_\Lambda-E_{-\Lambda})\frac{[ip(\phi)]^n}{n!}g$$

because $E_\Lambda-E_{-\Lambda}$ is bounded. Also, $E_\Lambda-E_{-\Lambda}$ commutes with $[ip(\phi)]^n/n!$, and $p(\phi)$ is bounded on $(E_\Lambda-E_{-\Lambda})\mathfrak{S}$, so

$$\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}(E_\Lambda-E_{-\Lambda})$$

converges uniformly to

$$e^{ip(\phi)}(E_\Lambda-E_{-\Lambda})=(E_\Lambda-E_{-\Lambda})e^{ip(\phi)}.$$

Therefore

$$(E_\Lambda-E_{-\Lambda})\sum_{n=0}^{\infty}\frac{[ip(\phi)]^n}{n!}g=(E_\Lambda-E_{-\Lambda})e^{ip(\phi)}g$$

for all Λ. But $E_\Lambda-E_{-\Lambda}\to I$ as $\Lambda\to\infty$.] Therefore

$$e^{ip(\phi)}q(\phi_1)f=q(\phi_1)e^{ip(\phi)}f+e^{ip(\phi)}\,\mathrm{Re}(\phi,\phi_1)f.$$

Therefore

$$[e^{ip(\phi)}q(\phi_1)]_o=\{[q(\phi_1)+\mathrm{Re}(\phi,\phi_1)]e^{ip(\phi)}\}_o,$$

and

$$[e^{ip(\phi)}q(\phi_1)]_o\subseteq[q(\phi_1)+\mathrm{Re}(\phi,\phi_1)]e^{ip(\phi)}.$$

But

$$[\{e^{ip(\phi)}q(\phi_1)\}_o]^{\sim}=e^{ip(\phi)}[q(\phi_1)_o]^{\sim}=e^{ip(\phi)}q(\phi_1),$$[27]

and $[q(\phi_1)+\mathrm{Re}(\phi,\phi_1)]e^{ip(\phi)}$ is already closed, so

$$e^{ip(\phi)}q(\phi_1)\subseteq[q(\phi_1)+\mathrm{Re}(\phi,\phi_1)]e^{ip(\phi)},$$

in other words,

$$e^{ip(\phi)}q(\phi_1)e^{-ip(\phi)}\subseteq q(\phi_1)+\mathrm{Re}(\phi,\phi_1).$$

Since both sides are self-adjoint they must be equal.

Corollary.[28] $e^{ip(\phi)}C(\phi_1)e^{-ip(\phi)}=C(\phi_1)+(\phi_1,\phi)/\sqrt{2}$, and

$$e^{ip(\phi)}C^*(\phi_1)e^{-ip(\phi)}=C^*(\phi_1)+(\phi,\phi_1)/\sqrt{2}.$$

Proof.

$$C(\phi_1)=[q(\phi_1)-ip(\phi_1)]^{\sim}/\sqrt{2}=[q(\phi_1)-iq(i\phi_1)]^{\sim}/\sqrt{2},$$

so

$$\begin{aligned}e^{ip(\phi)}C(\phi_1)e^{-ip(\phi)}&=[q(\phi_1)+\mathrm{Re}(\phi,\phi_1)-iq(i\phi_1)-i\,\mathrm{Re}(\phi,i\phi_1)]^{\sim}/\sqrt{2}\\&=C(\phi_1)+[\mathrm{Re}(\phi,\phi_1)+i\,\mathrm{Re}i(\phi,\phi_1)]/\sqrt{2}\\&=C(\phi_1)+[\mathrm{Re}(\phi_1,\phi)+i\,\mathrm{Im}(\phi_1,\phi)]/\sqrt{2}.\end{aligned}$$

Lemma 5.

$$e^{-ip(\phi)}\phi^{(0)}=e^{-(\phi,\phi)/4}\sum_{n=0}^{\infty}\phi^{(n)}/(2^n n!)^{\frac{1}{2}}.$$

Proof.

Let

$$\{\phi_i\}_{i=1}^{\infty}$$

[25] Footnote 12, p. 232, Th. 11.

[26] Footnote 12, p. 229.

[27] $[q(\phi_1)_0]^{\sim}=q(\phi_1)$ by the proof of Th. 10 on p. 231 of footnote 12.

[28] S. Tomonaga, Progr. Theoret. Phys. (Kyoto) **2**, 6 (1947); especially p. 10, Eq. (3.8).

be an orthonormal basis of $\mathfrak{R}$ such that $i>1$ implies $\phi_i \perp \phi$.

The set of all $C(\phi_{i_1})\cdots C(\phi_{i_n})\phi^{(0)}$ is an orthogonal basis of $\mathfrak{S}$.[29]

If $i_k>1$ for some k, then

$$(e^{-ip(\phi)}\phi^{(0)}, C(\phi_{i_1})\cdots C(\phi_{i_n})\phi^{(0)}) = (e^{-ip(\phi)}C^*(\phi_{i_k})\phi^{(0)}, C(\phi_{i_1})\cdots C(\phi_{i_{k-1}}) \times C(\phi_{i_{k+1}})\cdots C(\phi_{i_n})\phi^{(0)})$$

because the $C(\phi_{i_j})$ commute on $\mathfrak{S}_0$,[30] and $C^*(\phi_{i_k})$ commutes with $e^{-ip(\phi)}$ by the corollary to lemma 4. But $C^*(\phi_{i_k})\phi^{(0)}=0$.[29] Therefore

$$(e^{-ip(\phi)}\phi^{(0)}, C(\phi_{i_1})\cdots C(\phi_{i_n})\phi^{(0)})=0$$

when it is not the case that all $i_j=1$. Therefore

$$e^{-ip(\phi)}\phi^{(0)} = \sum_{n=0}^{\infty} \alpha_n C(\phi_1)^n\phi^{(0)},$$

where

$$\alpha_n = (e^{-ip(\phi)}\phi^{(0)}, C(\phi_1)^n\phi^{(0)})\|C(\phi_1)^n\phi^{(0)}\|^{-2}.$$

But

$$(e^{-ip(\phi)}\phi^{(0)}, C(\phi_1)^n\phi^{(0)}) = (\phi^{(0)}, e^{ip(\phi)}C(\phi_1)^n\phi^{(0)}) = (e^{-ip(\phi)}[(\phi,\phi_1)/\sqrt{2}]^n\phi^{(0)},\phi^{(0)})$$

by repeated use of the corollary to lemma 4 and the fact that $C^*(\phi_1)\phi^{(0)}=0$. So

$$e^{-ip(\phi)}\phi^{(0)} = (e^{-ip(\phi)}\phi^{(0)},\phi^{(0)}) \sum_{n=0}^{\infty} \left[\frac{(\phi,\phi_1)}{\sqrt{2}}\right]^n \frac{C(\phi_1)^n\phi^{(0)}}{\|C(\phi_1)^n\phi^{(0)}\|^2}.$$

By linearity[31] we have $(\phi,\phi_1)C(\phi_1)=C[(\phi,\phi_1)\phi_1]$; also[29] we have $\|C(\phi_1)^n\phi^{(0)}\|^2=n!$, so

$$e^{-ip(\phi)}\phi^{(0)} = (e^{-ip(\phi)}\phi^{(0)},\phi^{(0)}) \sum_{n=0}^{\infty} \frac{C[(\phi,\phi_1)\phi_1]^n\phi^{(0)}}{\sqrt{2}^n n!}$$

$$= (e^{-ip(\phi)}\phi^{(0)},\phi^{(0)}) \sum_{n=0}^{\infty} \frac{C(\phi)^n\phi^{(0)}}{\sqrt{2}^n n!} \quad (\text{since } \phi \| \phi_1)$$

$$= (e^{-ip(\phi)}\phi^{(0)},\phi^{(0)}) \sum_{n=0}^{\infty} \frac{\phi^{(n)}}{(2^n n!)^{\frac{1}{2}}}.$$[29]

Now define

$$u(\tau) = (e^{-i\tau p(\phi)}\phi^{(0)},\phi^{(0)}).$$

u is differentiable[32] since $\phi^{(0)}\in\mathfrak{D}p(\phi)$, and

$$u'(\tau) = -(e^{-i\tau p(\phi)}ip(\phi)\phi^{(0)},\phi^{(0)}) = (e^{-i\tau p(\phi)}C(\phi)\phi^{(0)},\phi^{(0)})/\sqrt{2} = ([C(\phi)-(\phi,\tau\phi)/\sqrt{2}]e^{-i\tau p(\phi)}\phi^{(0)},\phi^{(0)})/\sqrt{2}$$

by the corollary to lemma 4. So

$$u'(\tau) = [e^{-i\tau p(\phi)}\phi^{(0)}, C^*(\phi)\phi^{(0)}]/\sqrt{2} - \tau(\phi,\phi)^{\frac{1}{2}}(e^{-i\tau p(\phi)}\phi^{(0)},\phi^{(0)});$$

i.e., since the first summand is zero, we have shown $u'(\tau)=-\tau(\phi,\phi)^{\frac{1}{2}}u(\tau)$, with the boundary condition $u(0)=(\phi^{(0)},\phi^{(0)})=1$. Therefore $u(\tau)=e^{-(\phi,\phi)\tau^2/4}$, and $(e^{-ip(\phi)}\phi^{(0)},\phi^{(0)})=u(1)=e^{-(\phi,\phi)/4}$.

Corollary 1. $(e^{-ip(\phi)}\phi^{(0)},\phi^{(0)})=e^{-(\phi,\phi)/4}$

Corollary 2. $e^{ip(\phi)}\mathfrak{S}_0\subset\mathfrak{D}d\Gamma(I)$.

Proof.

Let $\mathfrak{R}=\mathfrak{M}_\phi\oplus\mathfrak{M}_\phi^{\perp}$, where $\mathfrak{M}_\phi$ is the one-dimensional subspace spanned by ϕ (which we may assume $\neq 0$). Then, under the canonical isomorphism

$$\mathfrak{S}(\mathfrak{R})\cong\mathfrak{S}(\mathfrak{M}_\phi)\otimes\mathfrak{S}(\mathfrak{M}_\phi^{\perp}),$$

we have

$$e^{ip(\phi)}\cong e^{ip(\phi)}\otimes I_2,$$

$$\mathfrak{S}(\mathfrak{R})_o\cong[\mathfrak{S}(\mathfrak{M}_\phi)\otimes\mathfrak{S}(\mathfrak{M}_\phi^{\perp})]_o\subset\mathfrak{S}(\mathfrak{M}_\phi)_o\otimes\mathfrak{S}(\mathfrak{M}_\phi^{\perp}),$$

and

$$d\Gamma(I)\cong[d\Gamma(P_\phi)\otimes I_2+I_1\otimes d\Gamma(P_\phi^{\perp})]^{\sim}$$

(by the corollary to lemma 1)

$$\supseteq d\Gamma(P_\phi)\otimes I_2+I_1\otimes d\Gamma(P_\phi^{\perp}).$$

Therefore, we may assume $\mathfrak{R}$ one-dimensional (i.e., $=\mathfrak{M}_\phi$).

Since $\mathfrak{S}(\mathfrak{R})_o$ now consists of linear combinations $\alpha_0\phi^{(0)}+\cdots+\alpha_m\phi^{(m)}$, it will be sufficient to prove $e^{ip(\phi)}\phi^{(n)}\in\mathfrak{D}d\Gamma(I)$.

But $\phi^{(n)}=n!^{-\frac{1}{2}}C(\phi)^n\phi^{(0)}$, so

$$e^{ip(\phi)}\phi^{(n)} = n!^{-\frac{1}{2}}[C(\phi)+(\phi,\phi)/\sqrt{2}]^n e^{ip(\phi)}\phi^{(0)}$$

by the corollary to lemma 4, and it remains only to show $C(\phi)^{(n)}e^{ip(\phi)}\phi^{(0)}\in\mathfrak{D}d\Gamma(I)$, i.e.,

$$\sum_{k=0}^{\infty}\left\|(n+k)\frac{e^{-(\phi,\phi)/4}}{(2^k k!)^{\frac{1}{2}}}C(\phi)^n(-\phi)^{(k)}\right\|^2 = e^{-(\phi,\phi)/2}\sum_{k=0}^{\infty}\frac{(n+k)^2}{2^k k!}\frac{(k+n)!}{k!}\|\phi\|^{2(n+k)} < \infty.$$

Convergence here is assured by the ratio test.

Theorem 1.[33] If H is self-adjoint and $\phi\in\mathfrak{D}H$, then

$$[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi]^{\sim} = e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}.$$

Proof.

If H is the projection of $\mathfrak{R}$ onto the one-dimensional subspace spanned by the normalized vector ϕ_1, then

[29] Footnote 12, p. 228, Lemma 2.
[30] Footnote 12, p. 230, Th. 8.
[31] Footnote 12, Sec. 2, p. 225.
[32] M. H. Stone, Ann. Math. 33, 647 (1932), Th. D.

[33] The formula $H_{\text{total}}=UH_{\text{free}}U^{-1}$ is due to C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. 23, No. 1, 1 (1945), Eq. (65). For the special form it takes in theorem 1, see p. 46 of G. Wentzel[10]; also Eq. (14.21), p. 82 of K. O. Friedrichs[10]; or Eq. (7-40), p. 126 of J. M. Jauch and F. Rohrlich.[10]

$d\Gamma(H)=C(\phi_1)C^*(\phi_1)$,[34] so

$$e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}$$
$$=[e^{ip(\phi)}C(\phi_1)e^{-ip(\phi)}][e^{ip(\phi)}C^*(\phi_1)e^{-ip(\phi)}]$$
$$=[C(\phi_1)+(\phi_1,\phi)/\sqrt{2}][C^*(\phi_1)+(\phi,\phi_1)/\sqrt{2}]$$

by the corollary to lemma 4.

Since

$$\mathfrak{D}[C(\phi_1)+(\phi_1,\phi)/\sqrt{2}][C^*(\phi_1)+(\phi,\phi_1)/\sqrt{2}]$$
$$=\mathfrak{D}C(\phi_1)C^*(\phi_1)\subset\mathfrak{D}C(\phi_1)=\mathfrak{D}C^*(\phi_1),^{29}$$

we have

$$\mathfrak{D}[C(\phi_1)+(\phi_1,\phi)/\sqrt{2}][C^*(\phi_1)+(\phi,\phi_1)/\sqrt{2}]$$
$$=\mathfrak{D}[C(\phi_1)C^*(\phi_1)]+[(\phi,\phi_1)/\sqrt{2}]C(\phi_1)$$
$$+[(\phi_1,\phi)/\sqrt{2}]C^*(\phi_1)+\tfrac{1}{2}(\phi_1,\phi)(\phi,\phi_1),$$

so

$$e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}$$
$$=C(\phi_1)C^*(\phi_1)+[(\phi,\phi_1)/\sqrt{2}]C(\phi_1)$$
$$+[(\phi_1,\phi)/\sqrt{2}]C^*(\phi_1)+\tfrac{1}{2}(\phi_1,\phi)(\phi,\phi_1)$$
$$=d\Gamma(H)+(\{C[(\phi,\phi_1)\phi_1]+C^*[(\phi,\phi_1)\phi_1]\}/\sqrt{2})$$
$$+\tfrac{1}{2}((\phi,\phi_1)\phi_1,\phi)$$
$$=d\Gamma(H)+\{[C(H\phi)+C^*(H\phi)]/\sqrt{2}\}+\tfrac{1}{2}(H\phi,\phi)$$
$$\subseteq d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi).$$

Since $e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}$ is maximal, the theorem is true when H is such a projection.

Now let H be an arbitrary projection. By means of the canonical isomorphism

$$\mathfrak{S}\{(H\mathfrak{R})\oplus[(I-H)\mathfrak{R}]\}\cong\mathfrak{S}(H\mathfrak{R})\otimes\mathfrak{S}[(I-H)\mathfrak{R}],$$

with $e^{ip(\phi)}\cong e^{ip(H\phi)}\otimes e^{[ip(I-H)\phi]}$, we can use lemma 1, and then its corollary, to reduce our problem to the case when H is the identity; i.e., we need only prove

$$[d\Gamma(I)+q(\phi)+\tfrac{1}{2}(\phi,\phi)]^\sim=e^{ip(\phi)}d\Gamma(I)e^{-ip(\phi)}.$$

Here we use the canonical isomorphism

$$\mathfrak{S}\{(P_\phi\mathfrak{R})\oplus[(I-P_\phi)\mathfrak{R}]\}\cong\mathfrak{S}(P_\phi\mathfrak{R})\otimes\mathfrak{S}[(I-P_\phi)\mathfrak{R}],$$

with $e^{ip(\phi)}\cong e^{ip(\phi)}\otimes I_2$, and lemma 1 followed by its corollary, to reduce the problem to the one-dimensional case which has already been considered.

So the theorem is true for arbitrary projections.

Now let $H=\alpha_1P_1+\cdots+\alpha_mP_m$, where the P_1 are orthogonal projections and the α_1 are real numbers ≥ 1. Then, by linearity, by the previous paragraph, and by lemma 1, the theorem is true here also.

Now let H be any self-adjoint operator $\geq I$. By the spectral theorem, there exists a sequence $H_k\uparrow H$ which, by the previous paragraph, obey the conditions of lemma 3. By lemma 2, H obeys the remaining conditions, so we can assert theorem 1 for self-adjoint $H\geq I$.

Now let $H=\int_0^\infty\lambda dE_\lambda$ be any self-adjoint operator ≥ 0. We know that the theorem is true for I and HE_1+I (since both are $\geq I$), so

$$e^{ip(\phi)}d\Gamma(HE_1+I)e^{-ip(\phi)}-e^{ip(\phi)}d\Gamma(I)e^{-ip(\phi)}$$
$$=[d\Gamma(HE_1+I)+q(HE_1\phi+\phi)+\tfrac{1}{2}(HE_1\phi+\phi,\phi)]^\sim$$
$$-[d\Gamma(I)+q(\phi)+\tfrac{1}{2}(\phi,\phi)]^\sim.$$

Since $[d\Gamma(HE_1+I)-d\Gamma(I)]^\sim=d\Gamma(HE_1)$, we can say

$$e^{ip(\phi)}d\Gamma(HE_1)e^{-ip(\phi)}$$
$$\supseteq[d\Gamma(HE_1+I)+q(HE_1\phi+\phi)+\tfrac{1}{2}(HE_1\phi+\phi,\phi)]^\sim$$
$$-[d\Gamma(I)+q(\phi)+\tfrac{1}{2}(\phi,\phi)]^\sim$$
$$\supseteq[d\Gamma(HE_1)+q(HE_1\phi)+\tfrac{1}{2}(HE_1\phi,\phi)]_o,$$

and

$$e^{ip(\phi)}d\Gamma(HE_1)e^{-ip(\phi)}$$
$$\supseteq[\{d\Gamma(HE_1)+q(HE_1\phi)+\tfrac{1}{2}(HE_1\phi,\phi)\}_o]^\sim.$$

To prove the reverse inclusion, let

$$f\in\mathfrak{D}e^{ip(\phi)}d\Gamma(HE_1)e^{-ip(\phi)},$$

and

$$e^{-ip(\phi)}f=\sum_{k=0}^{\infty}f_k'\in\mathfrak{D}d\Gamma(HE_1).$$

Then $h_m=f_0'\oplus\cdots\oplus f_m'\oplus 0\oplus\cdots\in\mathfrak{S}_0$, and $h_m\to e^{-ip(\phi)}f$. Since $\mathfrak{D}d\Gamma(I)\subset\mathfrak{D}d\Gamma(HE_1)$ (because $0\leq HE_1\leq 1$) and $\mathfrak{D}d\Gamma(I)\subset\mathfrak{D}C(HE_1\phi)=\mathfrak{D}C^*(HE_1\phi)$,[29] we have

$$e^{ip(\phi)}h_m\in\mathfrak{D}[\{d\Gamma(HE_1)+q(HE_1\phi)+\tfrac{1}{2}(HE_1\phi,\phi)\}_o]^\sim$$

by corollary 2 to lemma 5.

Further, $e^{ip(\phi)}h_m\to f$ and

$$[\{d\Gamma(HE_1)+q(HE_1\phi)+\tfrac{1}{2}(HE_1\phi,\phi)\}_o]^\sim e^{ip(\phi)}h_m$$
$$=[e^{ip(\phi)}d\Gamma(HE_1)e^{-ip(\phi)}]e^{ip(\phi)}h_m$$
(from the foregoing inclusion)
$$=e^{ip(\phi)}d\Gamma(HE_1)h_m\to e^{ip(\phi)}d\Gamma(HE_1)e^{-ip(\phi)}f$$
[since $e^{-ip(\phi)}f\in\mathfrak{D}d\Gamma(HE_1)$].

So, by the closure of

$$[\{d\Gamma(HE_1)+q(HE_1\phi)+\tfrac{1}{2}(HE_1\phi,\phi)\}_o]^\sim,$$

f is in its domain. Therefore

$$e^{ip(\phi)}d\Gamma(HE_1)e^{-ip(\phi)}$$
$$=[\{d\Gamma(HE_1)+q(HE_1\phi)+\tfrac{1}{2}(HE_1\phi,\phi)\}_o]^\sim.$$

Since $H(I-E_1)\geq I$, we already know

$$e^{ip(\phi)}d\Gamma[H(I-E_1)]e^{-ip(\phi)}$$
$$=[\{d\Gamma[H(I-E_1)]+q[H(I-E_1)\phi]$$
$$+\tfrac{1}{2}(H(I-E_1)\phi,\phi)\}_o]^\sim.$$

Combining these two results, we get

$$e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}$$
$$=[e^{ip(\phi)}d\Gamma(HE_1)e^{-ip(\phi)}+e^{ip(\phi)}d\Gamma\{H(I-E_1)\}e^{-ip(\phi)}]^\sim$$
$$=[[\{d\Gamma(HE_1)+q(HE_1\phi)+\tfrac{1}{2}(HE_1\phi,\phi)\}_o]^\sim$$
$$+[\{d\Gamma[H(I-E_1)]+q[H(I-E_1)\phi]$$
$$+\tfrac{1}{2}(H(I-E_1)\phi,\phi)\}_o]^\sim]^\sim$$
$$=[[\{d\Gamma(HE_1\oplus 0)+q(HE_1\phi\oplus 0)\}_o]^\sim$$
$$+[\{d\Gamma[0\oplus H(I-E_1)]+q[0\oplus H(I-E_1)\phi]\}_o]^\sim]^\sim$$
$$+\tfrac{1}{2}(H\phi,\phi),$$

[34] Footnote 12, p. 229, Lemma 3.

where $\mathfrak{R}$ has been decomposed into

$$\mathfrak{R}=(E_1\mathfrak{R})\oplus[(I-E_1)\mathfrak{R}].$$

Therefore, applying the corollary of lemma 1 separately to each summand, we have

$$\begin{aligned}
&e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}\\
&\quad\cong[[[\{d\Gamma(HE_1)+q(HE_1\phi)\}_o]^\sim\otimes I_2+I_1\otimes 0_2]^\sim\\
&\qquad+[0_1\otimes I_2+I_1\otimes[\{d\Gamma[H(I-E_1)]\\
&\qquad+q[H(I-E_1)\phi]\}_o]^\sim]^\sim]^\sim+\tfrac{1}{2}(H\phi,\phi)\\
&\quad=[[\{d\Gamma(HE_1)+q(HE_1\phi)\}_o]^\sim\otimes I_2\\
&\qquad+I_1\otimes[\{d\Gamma[H(I-E_1)]+q[H(I-E_1)\phi]\}_o]^\sim]^\sim\\
&\qquad+\tfrac{1}{2}(H\phi,\phi).
\end{aligned}$$

Now we use lemma 1 and then its corollary in order to get from $\mathfrak{S}(E_1\mathfrak{R})\otimes\mathfrak{S}[(I-E_1)\mathfrak{R}]$ back onto $\mathfrak{S}(\mathfrak{R})$:

$$\begin{aligned}
&e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}\\
&\qquad=[\{d\Gamma[HE_1\oplus H(I-E_1)]\\
&\qquad\quad+q[HE_1\phi\oplus H(I-E_1)\phi]\}_o]^\sim+\tfrac{1}{2}(H\phi,\phi),
\end{aligned}$$

or

$$e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}=[\{d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi\}_o]^\sim,$$

and the theorem is true for self-adjoint $H\geq 0$.

Finally, let $H=\int\lambda dE_\lambda$ be an arbitrary self-adjoint operator.

To finish the proof, we need only repeat the above usages of lemma 1 and its corollary with E_1 replaced by E_0.

(We have actually proven the slightly stronger theorem

$$[\{d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)\}_o]^\sim=e^{ip(\phi)}d\Gamma(H)e^{-ip(\phi)}.)$$

CONVERGENCE TO THE MØLLER WAVE OPERATOR

Theorem 2. If H is self-adjoint and $\phi\in\mathfrak{D}H$ and $e^{iHt}\phi$ goes weakly to zero, then

$$\exp\{i[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim t\}\exp[-id\Gamma(H)t]$$

goes weakly to $e^{-(\phi,\phi)/4}e^{ip(\phi)}$ as $t\to\pm\infty$.

Proof.

It is sufficient to show that

$$\begin{aligned}
&e^{-ip(\phi)}\exp\{i[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim t\}\\
&\qquad\times\exp[-id\Gamma(H)t]
\end{aligned}$$

goes weakly to $e^{-(\phi,\phi)/4}I$. But

$$\begin{aligned}
&e^{-ip(\phi)}\exp\{i[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim t\}\\
&\quad\times\exp[-id\Gamma(H)t]\\
&=\exp\{ie^{-ip(\phi)}[d\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim e^{ip(\phi)}t\}\\
&\quad\times e^{-ip(\phi)}\exp[-id\Gamma(H)t]\\
&=\exp[id\Gamma(H)t]e^{-ip(\phi)}\exp[-id\Gamma(H)t]\text{ by theorem 1}\\
&=\exp\{-i\exp[id\Gamma(H)t]p(\phi)\exp[-id\Gamma(H)t]\}\\
&=\exp[-ip(e^{iHt}\phi)],^{35}
\end{aligned}$$

[35] Footnote 12, p. 226, Th. 4.

so we need only prove that if ψ goes weakly to zero, and $\|\psi\|\to\|\phi\|$, then $e^{-ip(\psi)}$ goes weakly to $e^{-(\phi,\phi)/4}I$.

Because $e^{-ip(\psi)}$ is uniformly bounded for all ψ, and linear combinations of elements of the form

$$C(\phi_1)C(\phi_2)\cdots C(\phi_m)\phi^{(0)}$$

are strongly dense in $\mathfrak{S}$ (where $\phi_i\in\mathfrak{R}$ and $\phi^{(0)}\in\mathfrak{S}^{(0)}$, $\|\phi^{(0)}\|=1$), we need only prove

$$\begin{aligned}
&(e^{ip(\psi)}C(\phi_1)\cdots C(\phi_{m_1})\phi^{(0)},\\
&\quad C(\phi_{m_1+1})\cdots C(\phi_{m_1+m_2})\phi^{(0)})\longrightarrow e^{-(\phi,\phi)/4}\\
&\quad\times(C(\phi_1)\cdots C(\phi_{m_1})\phi^{(0)},C(\phi_{m_1+1})\cdots C(\phi_{m_1+m_2})\phi^{(0)}).
\end{aligned}$$

We can evaluate

$$\begin{aligned}
&(C(\phi_1)\cdots C(\phi_{m_1})\phi^{(0)},C(\phi_{m_1+1})\cdots C(\phi_{m_1+m_2})\phi^{(0)})\\
&\quad=(\phi^{(0)},C^*(\phi_{m_1})\cdots C^*(\phi_1)C(\phi_{m_1+1})\cdots C(\phi_{m_1+m_2})\phi^{(0)})
\end{aligned}$$

by using the commutation relations $[C^*(\phi_1),C(\phi_j)]^\sim=(\phi_j,\phi_i)I$[30] to shift all annihilation operators to the right where they are zero on $\phi^{(0)}$; so

$$(C(\phi_1)\cdots C(\phi_{m_1})\phi^{(0)},\ C(\phi_{m_1+1})\cdots C(\phi_{m_1+m_2})\phi^{(0)})$$

is 0 if $m_1\neq m_2$, and

$$=(\phi^{(0)},\phi^{(0)})\sum_{\text{permutations }p}\prod_{i=1}^{m_1}(\phi_{p(i)},\phi_{m_1+i})$$

if $m_1=m_2$.

If we try to evaluate

$$(e^{-ip(\psi)}C(\phi_1)\cdots C(\phi_{m_1})\phi^{(0)},C(\phi_{m_1+1})\cdots C(\phi_{m_1+m_2})\phi^{(0)})$$

in the same way, we get

$$(e^{-ip(\psi)}\phi^{(0)},\phi^{(0)})\textstyle\sum_p\prod_i(\phi_{p(i)},\phi_{m_1+i})\cdot\delta_{m_1,m_2}$$

plus a finite number of extra terms obtained by the commutation of $C(\phi_i)$ or $C^*(\phi_i)$ past $e^{-ip(\psi)}$. However, these extra terms all contain factors of the form (ϕ_i,ψ) or (ψ,ϕ_i) (by the corollary to lemma 4) which, in the weak limit as ψ goes to zero, must vanish.

Thus, since $(e^{-ip(\psi)}\phi^{(0)},\phi^{(0)})=e^{-(\psi,\psi)/4}$ (by corollary 1 to lemma 5) and $(\phi^{(0)},\phi^{(0)})=1$, the theorem is proven.

Define U by

$$\begin{aligned}
U(t_2,t_1)&=\exp[id\Gamma(H)t_2]\\
&\quad\times\exp\{[id\Gamma(H)+q(H\phi)+\tfrac{1}{2}(H\phi,\phi)]^\sim(t_1-t_2)\}\\
&\quad\times\exp[-id\Gamma(H)t_1].^{36}
\end{aligned}$$

(We will always assume H self-adjoint and $\phi\in\mathfrak{D}H$.)

$U(t_2,t_1)$ is a unitary operator such that $U(t_1,t_1)=I$, $U(t_1,t_2)=U(t_2,t_1)^{-1}$, and $U(t_3,t_2)U(t_2,t_1)=U(t_3,t_1)$.

Theorem 2 states that

$$\textit{weak limit } U(0,t)=e^{-(\phi,\phi)/4}e^{ip(\phi)}\quad\text{as}\quad t\to\pm\infty.$$

(Since * is weakly continuous, this implies

$$\textit{weak limit } U(t,0)=e^{-(\phi,\phi)/4}e^{-ip(\phi)}.)$$

[36] See J. M. Jauch and F. Rohrlich, footnote 10, p. 118; or see W. Brenig and R. Haag, Fortschr. Physik **7**, 183 (1959), especially p. 190.

Corollary 1.

$$U(t_2,t_1)=\exp[ip(e^{iHt_2}\phi)]\exp[-ip(e^{iHt_1}\phi)].$$

Proof.

Early in the proof of the theorem, we showed that

$$U(0,t_1)=\exp[ip(\phi)]\exp[-ip(e^{iHt_1}\phi)].$$

Therefore,

$$U(t_2,0)=U(0,t_2)^{-1}=\exp[ip(e^{iHt_2}\phi)]\exp[-ip(\phi)]$$

and

$$U(t_2,t_1)=U(t_2,0)U(0,t_1)$$
$$=\exp[ip(e^{iHt_2}\phi)]\exp[-ip(e^{iHt_1}\phi)].$$

Corollary 2. If *weak limit* $\psi=\psi'$ and $\|\psi\|^2\to\|\psi'\|^2+\alpha^2$, then *weak limit* $\exp[ip(\psi)]=\exp(-\alpha^2/4)\exp[ip(\psi')]$.

Proof.

$\mathfrak{R}\cong\mathfrak{M}_{\psi'}\oplus\mathfrak{M}_{\psi'^{\perp}}$ extends to $\mathfrak{S}(\mathfrak{R})\cong\mathfrak{S}(\mathfrak{M}_{\psi'})\otimes\mathfrak{S}(\mathfrak{M}_{\psi'^{\perp}})$ and $e^{ip(\psi)}\cong e^{ip(\psi_1)}\otimes e^{ip(\psi_2)}$ by the canonical isomorphism, where $\psi_2\perp\psi'$ and $\psi_1=\tau e^{i\theta}\psi'$ with $\tau=\|\psi_1\|/\|\psi'\|$. (If $\|\psi'\|=0$, then $\mathfrak{M}_{\psi'}$ does not occur.) So we need only prove $e^{ip(\psi_1)}\to e^{ip(\psi')}$ in $\mathfrak{S}(\mathfrak{M}_{\psi'})$ and

weak limit $\exp[ip(\psi_2)]=\exp(-\alpha^2/4)I$ in $\mathfrak{S}(\mathfrak{M}_{\psi'^{\perp}})$.

For the first,

$$e^{ip(\psi_1)}=\exp[ip(e^{i\theta}\psi')\tau]=\exp[ie^{id\Gamma(\theta I)}p(\psi')e^{-id\Gamma(\theta I)}\tau].^{35}$$

Therefore

$$e^{ip(\psi_1)}=e^{id\Gamma(\theta I)}e^{ip(\psi')\tau}e^{-id\Gamma(\theta I)}.$$

But $\|\psi_1\|\to\|\psi'\|$ and $e^{i\theta}\to 1$ (since *weak limit* $\psi_1=\psi'$ implies $\psi_1\to\psi'$ in one-dimensional $\mathfrak{M}_{\psi'}$), so

$$e^{ip(\psi')\tau}\to e^{ip(\psi')2^3} \quad\text{and}\quad e^{id\Gamma(\theta I)}\to I.$$

Therefore,

$$e^{id\Gamma(\theta I)}e^{ip(\psi')\tau}e^{-id\Gamma(\theta I)}\to Ie^{ip(\psi')}I^{-1},$$

i.e., $e^{ip(\psi_1)}\to e^{ip(\psi')}$.

For the second, we need only apply to $\mathfrak{S}(\mathfrak{M}_{\psi'^{\perp}})$ the latter part of the proof of theorem 2.

TIME-DEPENDENT SOURCE

For time-independent Hamiltonians we will need Weyl's bounded version of the commutation relations, in the form given them by Segal[37]:

Proposition.

$$\exp[ip(\phi_1)]\exp[ip(\phi_2)]$$
$$=\exp[ip(\phi_1+\phi_2)]\exp[i\tfrac{1}{2}\operatorname{Im}(\phi_1,\phi_2)].$$

Proof.

By the corollary to lemma 4, $e^{ip(\phi_1)}e^{ip(\phi_2)}$ and $e^{ip(\phi_1+\phi_2)}$ have the same commutation relations with any $C(\phi)$. But the set of all $C(\phi)$ is irreducible,[38] so $e^{ip(\phi_1)}e^{ip(\phi_2)}$ and $e^{ip(\phi_1+\phi_2)}$ can differ only by a multiplicative constant, $e^{ip(\phi_1)}e^{ip(\phi_2)}=ke^{ip(\phi_1+\phi_2)}$. It can be evaluated as follows:

$$(e^{ip(\phi_1)}e^{ip(\phi_2)}\phi^{(0)},\phi^{(0)})=k(e^{ip(\phi_1+\phi_2)}\phi^{(0)},\phi^{(0)}).$$

The left-hand side equals

$$(e^{ip(\phi_2)}\phi^{(0)},e^{-ip(\phi_1)}\phi^{(0)})$$
$$=\exp\{-[(\phi_1,\phi_1)+(\phi_2,\phi_2)]/4\}\sum_{n=0}^{\infty}(-\phi_2,\phi_1)^n2^{-n}/n!$$
$$=\exp\{-[(\phi_1,\phi_1)+(\phi_2,\phi_2)+2(\phi_2,\phi_1)]/4\}\text{ by lemma 5.}$$

The right-hand side equals

$$k\exp[-(\phi_1+\phi_2,\phi_1+\phi_2)/4]$$

by corollary 1 to lemma 5. Therefore

$$k=\exp\{-[(\phi_1,\phi_1)+(\phi_2,\phi_2)+2(\phi_2,\phi_1)]/4\}\times\exp[(\phi_1+\phi_2,\phi_1+\phi_2)/4]$$
$$=\exp\{[-2(\phi_2,\phi_1)+(\phi_2,\phi_1)+(\phi_1,\phi_2)]/4\}=\exp\{[(\phi_1,\phi_2)-(\phi_2,\phi_1)]/4\}$$
$$=\exp[i\tfrac{1}{2}\operatorname{Im}(\phi_1,\phi_2)]$$

Corollary

$$\exp[ip(\phi_1)]\cdots\exp[ip(\phi_n)]=\exp[ip(\phi_1+\cdots+\phi_n)]\times\exp[i\tfrac{1}{2}\operatorname{Im}\textstyle\sum_{1\le i\le j\le n}(\phi_i,\phi_j)].$$

We can expect $U(t,-t)$ to converge weakly[39] to a scalar multiple (Dyson's Z_2) of the S matrix, as $t\to\infty$.

From the proposition, and corollary 1 to theorem 2,

$$U(t,-t)=\exp\{ip[(e^{iHt}-e^{-iHt})\phi]\}\times\exp[-i\tfrac{1}{2}\operatorname{Im}(e^{2iHt}\phi,\phi)].$$

If *weak limit* $e^{iHt}\phi=0$ as $t\to\pm\infty$ (this will be the case, by the Riemann-Lebesgue lemma, if ϕ is in the absolutely continuous spectrum of H), then

$$\textit{weak limit}\ (e^{iHt}-e^{-iHt})\phi=0$$

also, and

$$\|(e^{iHt}-e^{-iHt})\phi\|^2=(e^{2iHt}\phi-\phi,e^{2iHt}\phi-\phi)\to 2\|\phi\|^2.$$

So, by corollary 2, *weak limit* $U(t,-t)=e^{-\frac{1}{2}(\phi,\phi)}I$.

$$[=\textit{weak limit}_{t_1\to-\infty}\ \textit{weak limit}_{t_2\to\infty}\ U(t_2,t_1)$$
$$=\textit{weak limit}_{t_2\to\infty}\ \textit{weak limit}_{t_1\to-\infty}\ U(t_2,t_1)\text{ by theorem 2}]$$

that is, the S matrix is trivial. No scattering has occurred because the state of the scatterer was not allowed to change.[40]

[37] I. E. Segal, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **31**, No. 12, 1 (1959), especially p. 16.

[38] Footnote 12, p. 231, Th. 9.

[39] See Sec. 3, Case I of R. Haag, Phys. Rev. **112**, 669 (1958); also Sec. 2, p. 205 of W. Brenig and R. Haag, Fortschr. Physik **7**, 183 (1959).

[40] G. Wentzel,[10] Sec. 7, pp. 42 and 47.

We will now allow the interaction Hamiltonian to vary with time and generalize U to include the case where $\phi=\phi_t$ is a function of t.

First let $t_1<t_2<\cdots<t_n$, and assume $\phi_t=\phi_{t_i}$ if $t_i\leq t<t_{i+1}$. Define $U(t_n,t_1)=U(t_n,t_{n-1})\cdots U(t_2,t_1)$. Then, by corollary 1 to theorem 2, and the corollary to the proposition,

$$U(t_n,t_1)=\exp\{ip\,[\sum_{i=1}^{n-1}(e^{iHt_{i+1}}-e^{iHt_i})\phi_{t_i}]\}$$
$$\cdot\exp\{-i\tfrac{1}{2}\,\mathrm{Im}\sum_{1\leq i\leq j\leq n-1}[(e^{iHt_{i+1}}-e^{iHt_i})\phi_{t_i},$$
$$(e^{iHt_{j+1}}-e^{iHt_j})\phi_{t_j}]\}$$
$$\cdot\exp[-i\tfrac{1}{2}\,\mathrm{Im}\sum_{i=1}^{n-1}(e^{iH(t_{i+1}-t_i)}\phi_{t_i},\phi_{t_i})].$$

By means of Pettis integrals[41] we can write

$$\sum_{i=1}^{n-1}(e^{iHt_{i+1}}-e^{iHt_i})\phi_{t_i}=\int_{t_1}^{t_n}e^{iHt}iH\phi_t dt$$

if all $\phi_t\in\mathfrak{D}H$. Therefore

$$U(t_n,t_1)=\exp\Big[ip\Big(\int_{t_1}^{t_n}e^{iHt}iH\phi_t dt\Big)\Big]$$
$$\times\exp\Big[-i\tfrac{1}{2}\,\mathrm{Im}\int_{t_1}^{t_n}\Big(\int_{t_1}^{t}e^{iHt'}iH\phi_{t'}dt',$$
$$e^{iHt}iH\phi_t\Big)dt\Big]\exp\Big[-i\tfrac{1}{2}\,\mathrm{Im}\int_{t_1}^{t_n}(iH\phi_t,\phi_t)dt\Big]$$

because, for fixed t_i and subdivision $t_i<t_i+\Delta<\cdots<t_i+k\Delta=t_{i+1}$ of the interval $[t_i,t_{i+1}]$, we have

$$\mathrm{Im}\sum_{j=1}^{k}(e^{iH(t_i+j\Delta)}\phi_{t_i+(j-1)\Delta},e^{iH[t_i+(j-1)\Delta]}\phi_{t_i+(j-1)\Delta})$$
$$=\mathrm{Im}k(e^{iH\Delta}\phi_{t_i},\phi_{t_i})=\mathrm{Im}k\Delta(\Delta^{-1}(e^{iH\Delta}-I)\phi_{t_i},\phi_{t_i})$$
$$=\mathrm{Im}(\Delta^{-1}(e^{iH\Delta}-I)\phi_{t_i},\phi_{t_i})$$
$$\times(t_{i+1}-t_i)\to\mathrm{Im}\int_{t_i}^{t_{i+1}}(iH\phi_t,\phi_t)dt,$$

since ϕ_t is constant in the interval and

$$\Delta^{-1}(e^{iH\Delta}-I)\phi_{t_i}\to iH\phi_{t_i}.^{32}$$

So, more generally, for any ϕ_t such that the integrals involved exist, we define

$$U(t_2,t_1)=\exp\Big[ip\Big(\int_{t_1}^{t_2}e^{iHt}iH\phi_t dt\Big)\Big]\exp-i\theta(t_2,t_1),$$

where $\theta(t_2,t_1)$ is the imaginary part of

$$\tfrac{1}{2}\int_{t_1}^{t_2}\Big(\int_{t_1}^{t}e^{iHt'}H\phi_t,dt',e^{iHt}H\phi_t\Big)dt$$
$$+\tfrac{1}{2}\int_{t_1}^{t_2}(iH\phi_t,\phi_t)dt.^{42}$$

If *weak limit* $\int_{-t}^{+t}e^{iH\tau}iH\phi_\tau d\tau=\int_{-\infty}^{+\infty}e^{iH\tau}iH\phi_\tau d\tau$,

and

$$\lim_{t\to\infty}\Big\|\int_{-t}^{+t}e^{iH\tau}iH\phi_\tau\Big\|$$

exists but is

$$>\Big\|\int_{-\infty}^{+\infty}e^{iH\tau}iH\phi_\tau d\tau\Big\|,$$

then (ignoring the phase factor),

$$\textit{weak limit}\,\exp\Big[ip\Big(\int_{-t}^{+t}e^{iH\tau}iH\phi_\tau d\tau\Big)\Big]$$
$$=Z_2\exp\Big[ip\Big(\int_{-\infty}^{+\infty}e^{iH\tau}iH\phi_\tau d\tau\Big)\Big]$$

by corollary 2 to theorem 2.

If

$$\lim_{t\to\infty}\Big\|\int_{-t}^{+t}e^{iH\tau}iH\phi_\tau d\tau\Big\|=\Big\|\int_{-\infty}^{+\infty}e^{iH\tau}iH\phi_\tau d\tau\Big\|$$

also, then

$$\exp\Big[ip\Big(\int_{-t}^{+t}e^{iH\tau}iH\phi_\tau d\tau\Big)\Big]\to$$
$$\exp\Big[ip\Big(\int_{-\infty}^{+\infty}e^{iH\tau}iH\phi_\tau d\tau\Big)\Big]$$

by the same corollary, because weak convergence of one unitary operator to another implies its strong convergence.

For example, suppose the interaction is switched on and off "adiabatically"[43] as follows: Let $\phi\in\mathfrak{D}H$ be constant, and $\phi_\tau=\phi e^{-\alpha|\tau|}$, $\alpha>0$. Then

$$\int_{-t}^{+t}e^{iH\tau}iH\phi_\tau d\tau$$
$$=\int_{-t}^{+t}e^{iH\tau-\alpha|\tau|}iH\phi d\tau=[iHe^{(iH+\alpha)\tau}(iH+\alpha)^{-1}]_{-t}^{0}\phi$$
$$+[iHe^{(iH-\alpha)\tau}(iH-\alpha)^{-1}]_{0}^{+t}\phi\to 2iH\alpha(H^2+\alpha^2)^{-1}\phi$$
as $t\to\infty$.

[41] E. Hille and R. S. Phillips, *Functional Analysis and Semi-Groups* (American Mathematical Society, Providence, Rhode Island, 1957), rev. ed., Chap. III, p. 77, Def. 3.7.1.

[42] See the lemma on p. 399 of J. M. Jauch and F. Rohrlich.[10]

[43] J. M. Jauch and F. Rohrlich,[10] p. 134; W. Brenig and R. Haag,[39] p. 191; K. O. Friedrichs,[10] p. 16.

[The validity of this formal integration is confirmed by applying Fubini's theorem to the spectral integral

$$\int_{-t}^{+t}\int_{-\infty}^{+\infty} e^{i\lambda\tau-\alpha|\tau|}i\lambda d(E_\lambda\phi,\psi)d\tau$$

for arbitrary ψ.] So

$$\exp\left[ip\left(\int_{-t}^{+t} e^{iH\tau}iH\phi_\tau d\tau\right)\right]\rightarrow$$

$$\exp\{ip[2iH\alpha(H^2+\alpha^2)^{-1}\phi]\} \quad \text{as} \quad t\rightarrow\infty.$$

Now $2iH\alpha(H^2+\alpha^2)^{-1}\phi\rightarrow 0$ as $\alpha\rightarrow 0$, so

$$\exp\{ip[2iH\alpha(H^2+\alpha^2)^{-1}\phi]\}\rightarrow I$$

as before except that strong convergence has replaced weak convergence and Z_2 has been eliminated.

Now to finish our earlier discussion of the neutral scalar meson field. Let the external source be represented by a real scalar function ρ of space-time. Since $\exp i(k_0t-\mathbf{k}\cdot\mathbf{x})$ is also invariantly defined, the integral $\int_\sigma \rho(t,\mathbf{x})\exp i(k_0t-\mathbf{k}\cdot\mathbf{x})d\sigma$ of their product over a fixed spacelike surface σ transforms like the three-volume element $d\sigma$. (Restrict ρ so that the integral exists and is, not only in $\mathfrak{R}$, but even in $\mathfrak{D}H^{-1}$.) Then q of that integral is the interaction Hamiltonian in the interaction picture, so,[44] in the Schrödinger picture $H_{\text{interaction}}=q(\hat{\rho}_\sigma)$ where

$$\hat{\rho}_\sigma(k_0,\mathbf{k})=\int_\sigma \rho(t,\mathbf{x})\exp(-i\mathbf{k}\cdot\mathbf{x})d\sigma.$$

The total Hamiltonian $[H_{\text{free}}+H_{\text{interaction}}]^\sim$ exists and is self-adjoint by theorem 1.

Addition of $H_{\text{interaction}}$ to H_{free} lowers the energy spectrum by $\frac{1}{2}(\hat{\rho}_\sigma,H^{-1}\hat{\rho}_\sigma)$ (theorem 1). If we parameterize our positive-frequency hyperboloid by $\mathbf{k}$, then $\hat{\rho}_\sigma$ is represented by $\hat{\rho}_\sigma[(\mathbf{k}^2+m^2)^{\frac{1}{2}},\mathbf{k}]$ in the Hilbert space of complex-valued functions of $\mathbf{k}$, square-integrable with respect to the measure $d^3\mathbf{k}/k_0$.[45] So

$$\tfrac{1}{2}(\hat{\rho}_\sigma,H^{-1}\hat{\rho}_\sigma)=\tfrac{1}{2}\int d^3\mathbf{k}\,|\hat{\rho}_\sigma[(\mathbf{k}^2+m^2)^{\frac{1}{2}},\mathbf{k}]|^2/k_0^2$$

$$=-\tfrac{1}{2}\int_\sigma\int_\sigma d^3\mathbf{x}d^3\mathbf{y}V(\mathbf{x}-\mathbf{y})\rho(t,\mathbf{x})\rho(t,\mathbf{y}),$$

where $V(\mathbf{x})=-e^{-m|\mathbf{x}|}/4\pi|\mathbf{x}|$ is the Yukawa potential.[46] We add this self-energy as a renormalization constant and redefine $H_{\text{total}}=[d\Gamma(H)+q(\hat{\rho}_\sigma)+\frac{1}{2}(\hat{\rho}_\sigma,H^{-1}\hat{\rho}_\sigma)I]^\sim$.

$U(t_2,t_1)$ can now be given a more invariant appearance.

$$\left(\int_{t_1}^{t_2} e^{iHt}iH\phi_t dt\right)(k_0,\mathbf{k})$$

$$=\left(\int_{t_1}^{t_2} e^{iHt}i\hat{\rho}_{\sigma(t)}dt\right)(k_0,\mathbf{k})$$

$$=i\int_{t_1}^{t_2}dt\int_{\sigma(t)}d^3\mathbf{x}\rho(t,\mathbf{x})e^{i(k_0t-\mathbf{k}\cdot\mathbf{x})},$$

so the transformation relating the field on two spacelike surfaces σ_1 and σ_2 is

$$\exp\left\{ip\left[i\int_{\sigma 1}^{\sigma 2} d^4x\rho(x)e^{i[(\cdot),\mathbf{x}]}\right]\right\}$$

in the interaction picture.

Two of the "catastrophes" of quantum field theory arise in the above formalism as follows. If $\hat{\rho}$ is not in $\mathfrak{D}H^{-1}$ (infrared catastrophe[47]), or if it is a Dirac delta function (ultraviolet catastrophe), then "$\|H^{-1}\hat{\rho}\|=\infty$" and the wave operator $\exp ip(H^{-1}\hat{\rho})$ of theorem 1 does not exist. Straightforward "completion of the square" does not correspond to a unitary transformation of Hilbert space.[48]

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[44] See Th. 4 on p. 226 of footnote 12.

[45] See p. 207 of Brenig and Haag,[39] or p. 24 of Wentzel.[10]

[46] See pp. 43–44 of Wentzel.[10]

[47] See pp. 75–76 of Friedrichs.[10]

[48] I. E. Segal, Trans. Am. Math. Soc. 88, 33 (1958), Example 2.

Synthetic Approach and Canonical Variables in a Nonlocal Field Theory*

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The analysis of the axiomatic structure of quantum field theory establishes what we call the synthetic approach. The translation in time is completely defined by its transformation function; it defines also canonical variables. The Hamiltonian is discussed at a later stage in order to establish the correspondence between this approach and the conventional one. An application is made to analyze Kristensen-Møller's theory of a nonlocal field. Its field variables are shown to be noncanonical; two field operators referring to two different points at the same time are not independent from each other, when the distance between the two points is of the order of the extension of the form factor; however, this fact does not disturb the calculation of the S matrix. The situation is clearly understood when the Kristensen-Møller field operators are compared with the corresponding canonical variables.

1. INTRODUCTION

THE purpose of this paper is to clarify the axiomatic structure of quantum field theory, especially when there is some form factor. The motivation behind this is to look for some field theoretical basis for a phenomenological approach in meson physics. In so doing, we make an approach in a synthetic way. In the traditional approach one starts with an assumed Lagrangian. In contrast to such an approach, here several properties of a field are taken for granted at the onset, and one tries to construct a theory which exhibits these properties with minimum number of assumptions.

The validity of quantum mechanics and the translation invariance together assert that there is a transformation function which transforms a state given at one time t, say, into the corresponding state at another time t'. It follows that one can solve the initial value problem. Also the canonical variables are explicitly defined by the transformation function. The existence of canonical variables, even when there is a form factor, was pointed out by Pauli.[1] The Hamiltonian is obtained uniquely when the transformation function is differentiated with respect to time.

It has been pointed out by the author[2] that the best way to handle the transformation function is to consider it in the exponential form. The arguments given there are amplified in the present paper. Our synthetic approach is applied to construct a transformation function with some form factor. In order to reduce arbitrariness in the new approach, the correspondence with the traditional approach is considered by looking at the form of the Hamiltonian. When the perturbation expansion is applied, it is found that two conditions determine the transformation function uniquely; these conditions are the Lorentz invariance of the S matrix and the assumption that no scattering is represented directly by the Hamiltonian when the local limit is taken. No systematic investigation of the self-action is attempted in the present paper.

The new approach is compared with the theory of Kristensen and Møller.[3] It is found that the solution of the Kristensen-Møller equation is not canonical; the commutator between two boson operators, for instance, for two different points at the same time does not vanish in general

$$[\varphi(x),\varphi(y)]|_{x_0=y_0}\neq 0. \tag{1}$$

It vanishes, however, when the time tends to positive or negative infinity. This means that it is complicated to list the complete set of independent variables at a finite time in the Kristensen-Møller theory. One must be critical of its use in a problem involving a bound state. On the other hand, the computation of the S matrix can be made disregarding the "noncanonicality." The theory of Bloch[4] applies here, if a bound state is discarded. The canonical variable does not present any difficulty of this kind, but the classical equation corresponding to it is not so simple as the Kristensen-Møller equation.

2. SYNTHETIC APPROACH

For the sake of a systematic exposition, the synthetic approach is to be divided into two steps, the kinematics and the dynamics. The kinematics is to prepare a set of states so complete that experimental information of any kind can be described. Mathematically, this is to define the Hilbert space which constitutes the basis for the whole theory. The current definition of a Hilbert space, which is developed to cover ordinary quantum mechanics, is not suitable to apply to quan-

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[1] W. Pauli, Nuovo cimento **10**, 648 (1953).

[2] S. Tani, Phys. Rev. **115**, 711 (1959); to be referred to as I. Some inadequate statement concerning the Lorentz invariance of the transformation function at a finite time is corrected at the end of Sec. 3 of the present paper; Phys. Rev. **117**, 1616(E) (1960).

[3] P. Kristensen and C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **27**, No. 7 (1952).

[4] C. Bloch, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **27**, No. 8 (1952).

tum field theory.[5] However, we can consistently state that the "Hilbert space" is defined, as a convention, when the manipulation with creation-annihilation operators of free particles is well defined.

2.1. Kinematics

Actually, most of the relevant kinematical considerations have been already made by various authors. A synthetic study was made by Foldy[6] with regard to the Lorentz transformation of the field equation for spin 0, $\frac{1}{2}$, or 1. The states of free particles as the representations of the Lorentz group were discussed by Haag.[7] The physical meaning of free particles was exhibited by many authors[8] in terms of asymptotic states. According to their physical meaning, creation-annihilation operators are to be introduced for every kind of stable particle, whether elementary or composite[9]; but one must note some subsidiary conditions.[10] Up to this point, the scheme of the present quantum field theory is quite consistent and general; we are not disturbed by the configuration where several particles approach close to each other.

2.2. Dynamics

We deal with flat spacelike surfaces, $t=$constant; this is not favorable to keep the Lorentz invariance of our theory, but it simplifies the arguments on the translational invariance without obscuring its general feature. Any state vector in the "Hilbert space" defined by the kinematics can be associated with one of these surfaces. At another time, the state of the system should be represented in the same "Hilbert space," but it may be laid in a different way because of the interaction among particles. Mathematically, there should be a well-defined transformation function.

Following the discussions exhibited in I, we put the transformation function from the time t' through t in the form

$$U(t,t')=\exp\left[(i/2)\int d^4x\epsilon(t,x_0)F(x)\right]\times\exp\left[(-i/2)\int d^4y\epsilon(t',y_0)F(y)\right]. \quad (2)$$

Here $\epsilon(a,b)$ denotes the step function

$$\epsilon(a,b)=\begin{cases}+1 & \text{for } a>b,\\ -1 & a<b.\end{cases} \quad (3)$$

The S matrix is to be defined by

$$S=\exp\left[i\int d^4xF(x)\right]. \quad (4)$$

The conditions to be satisfied by the operator $F(x)$ are as follows:

(1) $F(x)$ must be Hermitian to guarantee the unitarity.

(2) In view of Eq. (4), the energy conserving part of $F(x)$ must be Lorentz invariant.

(3) The S matrix defined by Eq. (4) must leave the vacuum and the one-particle states invariant.

(4) It is possible and convenient to choose $F(x)$ as a time-reversal invariant.

(5) The validity of Eq. (4) or (4′),

$$S=\lim_{\substack{t\to+\infty\\ t'\to-\infty}} U(t,t'), \quad (4')$$

requires that the matrix element of $F(x)$ is regular; operations with the delta functions and the principal value singularities must be well defined in momentum space.[11]

(6) When there exist a number of subsidiary conditions, $F(x)$ must be commutable with all of them.

Once the $F(x)$, which satisfies all the foregoing conditions, is given in terms of the creation-annihilation operators, all the information concerning the dynamics is implied by it. All the invariance properties known in quantum field theory can be incorporated with our formalism; especially the invariance against a translation in time is straightforward as seen from Eq. (2).

In a proper theory of the S matrix one should derive it from some specific assumption about the interaction such as is given by the field equation. After a specific assumption is introduced, only a smaller number of parameters than in the general framework for the S matrix should be at our disposal. We note here that the Hamiltonaian can be defined uniquely by differentiating the transformation function with respect to time. From the definition of the Hamiltonian

$$i(d/dt)U(t,t')=H(t)U(t,t'), \quad (5)$$

it is shown to be given by

$$H(t)=\int_{x_0=t} d^3x(F(x)+(1/2!)[F(x),-iG(t)]+(1/3!)\{[F(x),-iG(t)],-iG(t)\}+\cdots); \quad (6)$$

[5] Compare, e.g., K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields* (Interscience Publishers, Inc., New York, 1953), Part IV. Van Hove's paradox related to this point was discussed in I.

[6] L. L. Foldy, Phys. Rev. **102**, 568 (1956).

[7] R. Haag, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **29**, No. 12 (1955).

[8] F. J. Dyson, Phys. Rev. **75**, 1737 (1949); F. E. Low, *ibid.* **97**, 1392 (1955); H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo cimento **1**, 205 (1955).

[9] K. Nishijima, Phys. Rev. **111**, 995 (1958); W. Zimmermann, Nuovo cimento **10**, 597 (1958); R. Haag, Phys. Rev. **112**, 669 (1958).

[10] S. Tani, Phys. Rev. **117**, 252 (1960).

[11] A mathematically neat account on this point is given in a recent paper; see S. Tani (preprint).

the integration is extended over the three-dimensional surface, $x_0=t$. We have put

$$G(t)=\tfrac{1}{2}\int d^4y\epsilon(t,y_0)F(y). \tag{7}$$

As a result of the translational invariance, $H(t)$ is independent of t'.

In order to have a "theory" of the S matrix along the line mentioned previously, here we follow an analogy to the traditional approach. [We label channels according to the numbers and types of free field operators with which they are concerned. We name the fermion and the boson the nucleon and the pion, respectively, just as a matter of nomenclature. The channel where a single pion interacts with the nucleon current is labeled as $(NN\pi)$, for instance.] Now, we deal with a simple example and assume that there is no scattering directly represented in the Hamiltonian; $F(x)$ in all channels other than $(NN\pi)$ is given as a functional of the interaction introduced in $(NN\pi)$. For instance, Eq. (6) in the channel $(NN\pi\pi)$ reads

$$0=F_{NN\pi\pi}(x)+\tfrac{1}{2}[F_{NN\pi}(x),-iG_{NN\pi}(t)]_{NN\pi\pi} +\tfrac{1}{2}[F_{NN\pi\pi}(x),-iG_{NN\pi\pi}(t)]_{NN\pi\pi}+\cdots. \tag{8}$$

The subscripts to the commutator specify the part to be retained after the commutator calculation. One can see how the operator $F_{NN\pi\pi}(x)$, which yields the pion-nucleon scattering phase shift, is determined in terms of $F_{NN\pi}(x)$; it starts with the lowest-order Born approximation, the second term on the right-hand side of Eq. (8), and is corrected for the rescattering by the third term, and so forth.

On going into a further detail, Eq. (8) must be modified slightly in order to keep the S matrix Lorentz invariant. If the energy conserving part of $F(x)$ happens to violate the Lorentz invariance, the Hamiltonian is to be modified so that noninvariant terms cancel each other on both sides of Eq. (6). Accordingly, instead of Eq. (8), we calculate $F_{NN\pi\pi}$ starting from

$$F_{NN\pi\pi}(x)-H_{NN\pi\pi}(x) =\tfrac{1}{2}[F_{NN\pi}(x),iG_{NN\pi}(t)]_{NN\pi\pi} +\tfrac{1}{2}[F_{NN\pi\pi}(x),iG_{NN\pi\pi}(t)]_{NN\pi\pi}+\cdots. \tag{9}$$

Rules for making correction of this kind are exhibited in Sec. 3.

2.3. Remarks

We have specified only the channel into which the primary interaction is introduced; the form of $F_{NN\pi}$ is left open, and the present approach allows us to discuss the *quantization* of a field theory with a nonlocal form factor. The unitarity of the relevant transformations is guaranteed straightforwardly in our approach, while the Lorentz invariance can be established only by perturbation expansion. In this way, the feature of the present approach is complementary to the field theory with use of Heisenberg operators.[12]

Finally, a remark on the physical meaning of the representation used is due here. A representation, which we call the physical-particle representation, was discussed in I; all the effects of the self-action are eliminated in this representation. The construction of such a representation violates the crossing symmetry. We have to discriminate the two-pion creation by a nucleon from the pion-nucleon scattering, for instance. In view of this asymmetry in the physical-particle representation, we start with the interaction representation in constructing the operator $F(x)$. Once $F(x)$ is decided, one may go over to the physical-particle representation in order to check the interpretation of the S matrix.

3. CONSTRUCTION OF TRANSFORMATION FUNCTION WITH A FORM FACTOR

Let $\psi(x)$ and $\phi(x)$ denote a free field operator for a nucleon and a pion, respectively. At the first order of the perturbation expansion, we put

$$F^{(1)}(x)=F_{NN\pi}(x)=\int D(x',x'',x''') \times\delta(x-x'):\bar{\psi}(x')\phi(x'')\psi(x'''):. \tag{10}$$

Hereafter, we use the following abbreviation for the volume element in the integral

$$D(x',x'',x''')=d^4x'd^4x''d^4x'''f(x',x'',x'''), \tag{11}$$

with $f(x',x'',x''')$ denoting the form factor for the vertex. In Eq. (10) we have considered only the case where the meson coordinate x'' is identified with the argument x of F; this is the same as was considered by Pauli.[13] We ignore the possibility of having a subsidiary condition. The notation $:A:$ means to take the ordered form of the operator A according to Wick's rule.[14] The superscript denotes the order of the perturbation.

Discarding the mass operators, we have two terms at the second order,

$$F^{(2)}(x)=F_{NNNN}{}^{(2)}(x)+F_{NN\pi\pi}{}^{(2)}(x). \tag{12}$$

[12] One can find further references in the following paper: G. Källen and A. Wightman, Kgl. Danske Videnskab. Selskab, Mat.-fys. Skrifter **1**, No. 6 (1958). K. Nishijima [Phys. Rev. **119**, 485 (1960)] has studied the theory in which microscopic causality is taken for granted. His result is similar to ours in that perturbation expansion plays an essential role in the proof, although microscopic causality excludes any form factor.

[13] One can generalize Eq. (10) by interchanging x'' with x' or x''' and by taking a linear combination of these terms, but such a general expression is not necessary for our purpose.

[14] G. C. Wick, Phys. Rev. **80**, 268 (1950).

$F_{NNNN}{}^{(2)}$ obtains without introducing any $H_{NNNN}{}^{(2)}$. On applying Eq. (6) to the channel $(NNNN)$, we find

$$F_{NNNN}{}^{(2)}(x)=\int D(x',x'',x''')D(y',y'',y''')\times\delta(x-x'')\tfrac{1}{2}:\bar{\psi}(x')\bar{\psi}(y')\times\bar{D}(x''-y'')\psi(y''')\psi(x'''):. \quad (13)$$

This is Lorentz invariant. In the channel $(NN\pi\pi)$, we have

$$F_{NN\pi\pi}{}^{(2)}(x)-H_{NN\pi\pi}{}^{(2)}(x)=\int D(x',x'',x''')D(y',y'',y''')\cdot\tfrac{1}{4}\cdot\epsilon(x_0'',y_0'')\times[\delta(x-x'')+\delta(x-y'')]:\bar{\psi}(x')\phi(x'')\times S(x'''-y')\phi(y'')\psi(y'''):. \quad (14)$$

The ϵ function in Eq. (14) cannot be incorporated with an S function to give an $\bar{S}$ function. The corrected form for $F_{NN\pi\pi}{}^{(2)}$ is given by replacing $\epsilon(x_0'',y_0'')$ by $\epsilon(x_0''',y_0')$; we have

$$F_{NN\pi\pi}{}^{(2)}(x)=\int D(x',x'',x''')D(y',y'',y''')\tfrac{1}{2}[\delta(x-x'')+\delta(x-y'')]\times:\bar{\psi}(x')\phi(x'')\bar{S}(x'''-y')\phi(y'')\psi(y'''):. \quad (15)$$

It is noted that $F^{(2)}$ defined previously is time-reversal invariant. Introducing the phase matrix η by the exponent of the S matrix

$$S=\exp[2i\eta], \quad (16)$$

its second-order part is given by

$$\eta^{(2)}=\int D(x',x'',x''')D(y',y'',y''')\times[\tfrac{1}{2}:\bar{\psi}(x')\phi(x'')\bar{S}(x'''-y')\phi(y'')\psi(y'''):+\tfrac{1}{4}:\bar{\psi}(x')\bar{\psi}(y')\bar{D}(x''-y'')\psi(y''')\psi(x'''):]. \quad (17)$$

Up to the second order, the $F(x)$ is Lorentz invariant. It will be found that this is not true any more at the third order. Even in the local limit, only the energy conserving part of $F(x)$ is Lorentz invariant. Since we do not go beyond the second order in the analysis of the Kristensen-Møller equation, we only give the result without proof. $H^{(3)}$ is defined uniquely when we require it to vanish in the local limit. This requirement is legitimate, because $H^{(3)}$ becomes necessary because of the retardation effect within the form factor.

4. ANALYSIS OF KRISTENSEN-MØLLER'S EQUATION

The field equations proposed by Kristensen and Møller are given in our example by

$$(-\Box+m^2)\varphi(x)=\int\bar{\chi}(x')\delta(x-x'')\chi(x''')D(x',x'',x'''), \quad (18)$$

$$[\gamma(\partial/\partial x)+M]\chi(x)=\int\delta(x-x')\varphi(x'')\chi(x''')D(x',x'',x'''), \quad (18')$$

$$-[\partial\bar{\chi}(x)/\partial x]\gamma+M\bar{\chi}(x)=\int\bar{\chi}(x')\varphi(x'')\delta(x-x''')D(x',x'',x'''). \quad (18'')$$

We solve these equations by perturbation calculations. The solution depends on the boundary condition. As was shown in I, it is sufficient to solve the equation under the standing wave boundary condition. The relation among φ operators under different boundary conditions is given by Eq. (19), where the suffixes, r, a, and s, denote the out-going wave, the in-coming wave, and the standing wave solutions, respectively;

$$\exp[i\eta]\varphi_r\exp[-i\eta]=\exp[-i\eta]\varphi_a\exp[i\eta]=\varphi_s. \quad (19)$$

The φ_s is obtained by performing the iteration with the equation

$$\varphi_s(x)=\tfrac{1}{2}\{\exp[-i\eta]\phi(x)\cdot\exp[i\eta]+\exp[i\eta]\phi(x)\cdot\exp[-i\eta]\}+\int\bar{D}(x-x'')\bar{\chi}_s(x')\chi_s(x''')D(x',x'',x'''). \quad (20)$$

On the other hand, φ_r is obtained by working with

$$\varphi_r(x)=\phi(x)+\int[\bar{D}(x-x'')+\tfrac{1}{2}D(x-x'')]\bar{\chi}_r(x')\times\chi_r(x''')D(x',x'',x'''). \quad (20')$$

Explicitly written down, φ_s is found as

$$\varphi_s(x)=\phi(x)+\int D(x',x'',x''')\bar{\Psi}(x')\bar{D}(x-x'')\psi(x''')+\int D(x',x'',x''')D(y',y'',y''')\times[\bar{\psi}(x')\bar{D}(x-x'')\bar{S}(x'''-y')\phi(y'')\psi(y''')+\bar{\psi}(x')\phi(x'')\bar{S}(x'''-y')\bar{D}(x-y'')\psi(y''')+\tfrac{1}{8}\bar{\psi}(x')D(x-x'')S(x'''-y')\phi(y'')\psi(y''')+\tfrac{1}{8}\bar{\psi}(x')\phi(x'')S(x'''-y')D(y''-x)\psi(y''')]. \quad (21)$$

Let us investigate the translational property of the φ_s. Since the translational property for a free field operator is straightforward, we try here to find a unitary transformation which transforms a free field operator into the corresponding Kristensen-Møller operator;

$$\phi(x) \rightarrow \varphi_s(x) = U(\varphi:x_0)^{-1}\phi(x)U(\varphi:x_0). \quad (22)$$

On putting the unitary transformation in the exponential form

$$U(\varphi:x_0) = \exp[iG(\varphi:x_0)], \quad (23)$$

$G(\varphi:x_0)$ is found to be given by

$$G(\varphi:x_0) = \tfrac{1}{2}\int \epsilon(x_0,x_0'')\bar{\psi}(x')\phi(x'')\psi(x''')D(x',x'',x''')$$
$$+\tfrac{1}{4}\int D(x',x'',x''')D(y',y'',y''')$$
$$\times[\epsilon(x_0,x_0'')+\epsilon(x_0,y_0'')]\bar{\psi}(x')\phi(x'')$$
$$\times S(x'''-y')\phi(y'')\psi(y'''). \quad (24)$$

In fact, there is no unitary transformation in the form of Eq. (22); instead of Eq. (22), we have to put

$$\varphi_s(x) = \exp[-iG(\varphi:x_0)]\cdot[\phi(x)+\Delta\varphi]$$
$$\cdot\exp[iG(\varphi:x_0)]. \quad (25)$$

$\Delta\varphi(x)$ is given by

$$\Delta\varphi(x) = \tfrac{1}{8}\int D(x',x'',x''')D(y',y'',y''')$$
$$\times[\epsilon(x_0''',y_0')-\epsilon(x_0'',y_0'')]$$
$$\times[\epsilon(x_0,x_0'')-\epsilon(x_0,y_0'')]$$
$$\times[\bar{\psi}(x')D(x-x'')S(x'''-y')\phi(y'')\psi(y''')$$
$$-\bar{\psi}(x')\phi(x'')S(x'''-y')D(x-y'')\psi(y''')]. \quad (26)$$

If it happens that there are plus signs in the second and the third brackets, instead of minus signs, $\Delta\varphi$ can be removed by a unitary transformation, namely, by modifying the $G(\varphi:x_0)$; however, this would cause an undesirable change in the S matrix. It is to be noted that the asymptotic form of $G(\varphi:x_0)$ as $x_0 \rightarrow \pm\infty$ coincides correctly with the corresponding term in $\pm\eta$. [The phase matrix η has been defined by Eqs. (4), (10), (16), and (17). Physically there should be no contribution from the first-order term, Eq. (10), but for the sake of direct comparison with Pauli's result we retain it formally.]

Similar calculations are performed with regard to χ. The transformation for χ_s is given by

$$\chi_s(x) = \exp[-iG(\chi:x_0)][\psi(x)+\Delta\chi]$$
$$\times\exp[iG(\chi:x_0)]. \quad (27)$$

$G(\chi:x_0)$ is given by

$$G(\chi:x_0)$$
$$= \tfrac{1}{2}\int D(x',x'',x''')\epsilon(x_0,x_0')\bar{\psi}(x')\phi(x'')\psi(x''')$$
$$+\tfrac{1}{8}\int D(x',x'',x''')D(y',y'',y''')[\epsilon(x_0,x_0')+\epsilon(x_0,y_0')]$$
$$\times:\bar{\psi}(x')\bar{\psi}(y')\bar{D}(x''-y'')\psi(y''')\psi(x'''):$$
$$+\tfrac{1}{8}\int D(x',x'',x''')D(y',y'',y''')$$
$$\times[2\epsilon(x_0,x_0')\epsilon(x_0''',y_0')+1-\epsilon(x_0,x_0')\epsilon(x_0,y_0')]$$
$$\times:\bar{\psi}(x')\phi(x'')S(x'''-y')\phi(y'')\psi(y''')\,:. \quad (28)$$

$\Delta\chi$ is given by

$$\Delta\chi(x) = \tfrac{1}{8}\int D(x',x'',x''')D(y',y'',y''')$$
$$\times[\epsilon(x_0'',y_0'')-\epsilon(x_0',y_0')][\epsilon(x_0,x_0')-\epsilon(x_0,y_0')]$$
$$\times S(x-x')\bar{\psi}(y')D(x''-y'')\psi(y''')\psi(x'''). \quad (29)$$

One can see that $G(\chi:x_0)$ is different from $G(\varphi:x_0)$, but its asymptotic limit as $x_0 \rightarrow \pm\infty$ gives exactly $\pm\eta$.

The effect of the $\Delta\varphi$ is shown when we calculate the commutator between φ_s for two different points with the same time coordinate

$$[\varphi_s(x),\varphi_s(y)]\,|_{x_0=y_0}$$
$$= \tfrac{1}{4}\int D(x',x'',x''')D(y',y'',y''')\bar{\psi}(x')S(x''-y')\psi(y''')$$
$$\times[\epsilon(x_0''',y_0')-\epsilon(x_0'',y_0'')]\cdot[\epsilon(x_0,x_0'')-\epsilon(x_0,y_0'')]$$
$$\times[D(y-x'')D(x-y'')-D(x-x'')D(y-y'')]. \quad (30)$$

This result is independent of the boundary condition, as one can check directly. The deviation of the commutator from its canonical form is a feature inherent in Kristensen-Møller's equation. One sees that the right-hand side of Eq. (30) vanishes either when one takes the local limit or when the time x_0 tends to the infinity.[15]

On the other hand, the canonical variables defined in the last section do not present any abnormality like Eq. (30). As for the φ operator, for instance, the canonical variable is given by

$$\varphi_c(x) = U(x_0)^{-1}\cdot\phi(x)\cdot U(x_0), \quad (31)$$

[15] The conclusion reached here seems to have been suggested by C. Hayashi [Progr. Theoret. Phys. (Kyoto) **10**, 538 (1953); **11**, 226 (1954)]. Unfortunately, the quantization adopted in his paper is quite different from what has been discussed here.

where the transformation function $U(x_0)$ has been given in the last section; from Eqs. (2), (10), (13), (15), and (24), we see that

$$U(x_0)=\exp\Big[iG(\varphi:x_0)+\frac{i}{4}\int D(x',x'',x''')\times D(y',y'',y''')\epsilon(x_0,x_0'')\,{:}\bar{\psi}(x')\bar{\psi}(y')\times\bar{D}(x''-y'')\psi(y''')\psi(x''')\Big]. \quad (32)$$

From Eqs. (32) and (25), we see that, if the noncanonical term $\Delta\varphi$ were discarded, the Kristensen-Møller operator φ_s and the canonical variable φ_c would coincide. As for the nucleon operator, two kinds of operators are connected by

$$\chi_s(x)=V(\chi:x_0)^{-1}\cdot[\chi_c(x)+\Delta\chi(x)+\cdots]V(\chi:x_0) \quad (33)$$

with the unitary transformation function $V(\chi:x_0)$ given by

$$V(\chi:x_0)=U(x_0)^{-1}\cdot\exp[iG(\chi:x_0)]. \quad (34)$$

Thus, if the noncanonical term $\Delta\chi$ were discarded, the χ_s and the χ_c would be connected through a unitary transformation. It is to be noted that $V(\chi:x_0)$ reduces to the identity and $\Delta\chi(x)$ vanishes if the time x_0 tends to the infinity; the Kristensen-Møller operator and the canonical variable coincide asymptotically. It is now clear that the noncanonical commutation relation

$$[\varphi_s(x),\chi_s(y)]|_{x_0=y_0}\neq 0 \quad (35)$$

cannot be brought under the canonical form by performing a unitary transformation on χ_s. Pauli calculated the commutator only up to the first order in the perturbation expansion and he did not bring up this point.

As remarked already, the translational property of both φ_s and χ_s is consistent with the definition of the S matrix, which is based on the property of a canonical variable. Consequently, the relation among the Kristensen-Møller operators under the different boundary conditions in Eq. (19) is identical with the corresponding one among canonical variables; the effect of the noncanonical terms is eliminated in the calculation of the S matrix. One must be critical of the use of Kristensen-Møller's theory, if there appears a bound state.

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Some Counting Theorems in the Theory of the Ising Model and the Excluded Volume Problem

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The problem of the exact enumeration of self-avoiding random walks on a lattice is studied and a theorem derived that enables the number of such walks to be calculated recursively from the number of a restricted class of closed graphs more easily enumerated than the walks themselves. The method of Oguchi for deriving a high-temperature expansion for the zero-field susceptibility of the Ising model is developed and a corresponding theorem enabling the successive coefficients to be calculated recursively from a restricted class of closed graphs deduced. The theorem relates the susceptibility to the configurational energy and enables the behavior of the antiferromagnetic susceptibility at the transition point to be inferred.

1. INTRODUCTION

IT is the purpose of this paper to investigate the configurational counting problem presented by the method of Oguchi[1] for deriving the high-temperature expansion of the zero-field susceptibility of the Ising model. This is one of a class of problems connected with the enumeration of linear graphs on a lattice which arise in the theory of cooperative assemblies above their transition point and which may be called high-temperature counting problems. A problem of very similar nature and which arises in the theory of long-chain polymers in dilute solution is the enumeration of nonself-intersecting walks on a lattice by a study of the topologically equivalent linear graph. The relation between the two problems was remarked by Oguchi and has recently been studied by Temperley[2] and Fisher and Sykes.[3] For our present purpose the two problems are conveniently studied together. We shall first develop a method of obtaining the numerical value of c_n, the number of self-avoiding walks of n steps on a given lattice, for small values of n. The method will then be modified to apply to the more complex enumeration problem presented by the coefficients of the susceptibility expansion.

Numerical results will be given for a number of plane and three-dimensional lattices. The preliminary application of this data to the polymer problem has been made by Fisher and Sykes,[3] where a bibliography is also given. For applications of the data on susceptibility expansions reference should be made to a review article by Domb[4] where an extensive bibliography is given. The interpretation of the data is to be discussed in detail in a subsequent paper.

2. ENUMERATION OF LONG CHAINS

For small values of n the number of nonself-intersecting walks of n steps, or as we shall call them chains, on a given lattice may be obtained by direct enumeration of all the possible types. By an obvious extension of the method developed by Wakefield[5] for the enumeration of polygons on the simple cubic lattice, the chains may be classified into space types. For example, on the simple quadratic lattice there are four possible space types of 3-chain, which we illustrate in Fig. 1, making a total contribution of $18N$ on a lattice of N sites, and since we require the number of chains from a fixed origin and each of these types could be walked in both directions, we have

$$Nc_3=36N \quad \text{or} \quad c_3=36.$$

The description of the possible types need not be by drawing, but since the number of chains increases rapidly with n, it is difficult to proceed very far by direct methods. For example, on the simple quadratic lattice there are 2 374 444 distinct walks of 14 steps, and since the maximum contribution of a space type on this lattice is $8N$, there cannot be fewer than 148 403 of these. To avoid this difficulty we require methods which obviate detailed enumeration of the chains.

We have approached the problem as follows. If a self-avoiding walk of $(n-1)$ steps on a lattice of coordination number q is continued in any of the $(q-1)=\sigma$ directions that avoid an immediate reversal, the result is either a self-avoiding walk of n steps or a walk with one self-intersection which can occur with one of the two topologically distinct linear graphs illustrated in Fig. 2. The graph (a) results from a self-intersection at r steps from the origin. We shall describe this as a "tadpole," and we shall denote the number of such graphs on a given lattice by $T_{r,s}$. As usual, this is to be understood as the number reckoned per site, the total number of distinct structures on a torus of N sites being $NT_{r,s}$. With this definition every

FIG. 1. The four possible space types of 3-chain on the simple quadratic lattice.

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[1] T. Oguchi, J. Phys. Soc. Japan. **6**, 31 (1951).
[2] H. N. V. Temperley, Phys. Rev. **103**, 1 (1956).
[3] M. E. Fisher and M. F. Sykes, Phys. Rev. **114**, 45 (1959).
[4] C. Domb, Advances in Phys. (to be published).
[5] A. J. Wakefield, Proc. Cambridge Phil. Soc. **47**, 419 (1951).

tadpole will be walked twice, the s steps of the "head" being walked once in each sense. The graph (b) results from a self-intersection at the origin. If p_n is the number of polygons per site, there are np_n polygons through a given point, and each will be walked in two senses. Thus

$$c_n=\sigma c_{n-1}-2\sum_{r=1}^{n-3} T_{r,n-r}-2np_n. \tag{1}$$

Equation (1) enables us to deduce c_n from c_{n-1} by enumerating the tadpoles and polygons of order n (the order of a lattice constant being the number of bonds it contains, e.g., the order of $T_{r,s}$ is $r+s$).

For example, by careful drawing it is possible to deduce the first six values of c_n on the simple quadratic lattice. To add four more is laborious, but with Eq. (1) this is achieved without further drawing, since the number of square-headed tadpoles of each order can quite easily be deduced by counting the number of ways a square head can be added to each walk of order four less. The other tadpoles required, those with hexagonal and octagonal heads, present no difficulty at this stage.

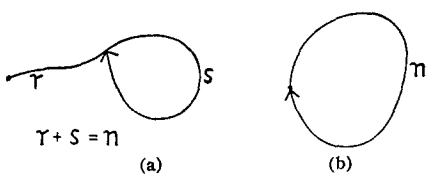


FIG. 2. Linear graphs that result from a self-intersection on the last step of a random walk: (a) tadpole, $T_{r,s}$; (b) polygon, p_n.

An obvious extension of this idea is to use the same technique to count the tadpoles. If we add a further step to the tail of the tadpole $T_{x-1,y}$, the product is either a new tadpole $T_{x,y}$ or one of the three products whose linear graphs are shown in Fig. 3, the number of these linear graphs per site being denoted by $(r,s,t)_d$, $p_r\cdot p_s$, $(r,s,t)_s$, respectively. We shall refer to (a)–(c) collectively as "generalized figure-eights." In the subclassification we have introduced the term "figure-eight star" to emphasize the fact that the lattice constant $(r,s,t)_s$ is a "star" in the notation of Riddell,[6] dumbbells and orthodox figure-eights being "trees."

The number of walks of order n can thus be made to depend on the number of generalized figure-eights and polygons of order n. The exact form of this dependence is not obvious and in the next section we shall derive a recurrence relation that enables the successive c_n to be calculated.

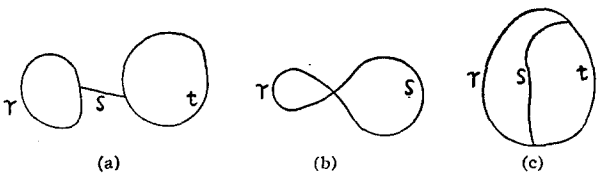


FIG. 3. Linear graphs that result from the intersection of a tadpole with its tail. (a) Dumbbell, $(r,s,t)_d$; (b) orthodox figure-eight, $p_r\cdot p_s$; (c) star figure-eight, $(r,s,t)_s$. $r+s+t=x+y=n$. *Note.* In (c) the distinction between the case of "s inside" and "s outside" (external bridge, internal bridge) is only meaningful for two-dimensional lattices. $(r,s,t)_s$ is to be taken as the total number of such structures.

3. CHAIN COUNTING THEOREM

We begin by examining the effect of adding one more step to the tail of the tadpole $T_{r-1,s}$, which we may do in σ ways if $r-1\neq 0$. For this case, we have

$$T_{r,s}=\sigma T_{r-1,s}-F_{r,s}, \tag{2a}$$

where $F_{r,s}$ is a linear sum of lattice constants[7] of order $r+s$ and of type (a), (b), or (c) of Fig. 3. If $r-1=0$, the tadpole reduces to the polygon p_s to which we may add a unit tail in $(\sigma-1)$ ways at any of s points to form $T_{1,s}$ or a star figure-eight [Fig. 3(c)],

$$T_{1,s}=s(\sigma-1)p_s-F_{1,s}, \tag{2b}$$

where $F_{1,s}$ is again a linear sum of lattice constants of order $s+1$.

From (2a) and (2b),

$$\sum_{r=1}^{n-3} T_{r,n-r}=\sigma\sum_{r=2}^{n-3} T_{r-1,n-r}+(n-1)(\sigma-1)p_{n-1}-\sum_{r=1}^{n-3} F_{r,n-r}. \tag{3}$$

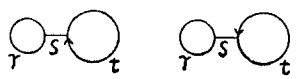
On replacing n by $n+1$ in (1) and subtracting σ times (1) from the result, the two summations that involve tadpoles cancel by virtue of (3), and we obtain

$$c_{n+1}-2\sigma c_n+\sigma^2 c_{n-1}=2np_n-2(n+1)p_{n+1}+2\sum_{r=1}^{n-2} F_{r,n-r+1}. \tag{4}$$

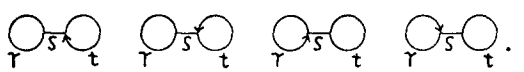
It remains to establish the form of the summation in (4), which is a linear sum in generalized figure-eights or order $(n+1)$. Dumbbells and orthodox figure-eights that occur in this sum will be examined together, an orthodox figure-eight $p_x\cdot p_y$ being regarded as the dumbbell $(x,0,y)_d$. In our notation $(r,s,t)_d\equiv(t,s,r)_d$,

[6] *Note.* "Stars" are connected graphs without a cutting point. "Trees" are connected graphs with one or more cutting points. A cutting point is a point where the graph could be cut into two or more separated graphs by cutting all the lines going to this point (Riddell[6a]). (a) R. J. Riddell, thesis, University of Michigan, 1951.

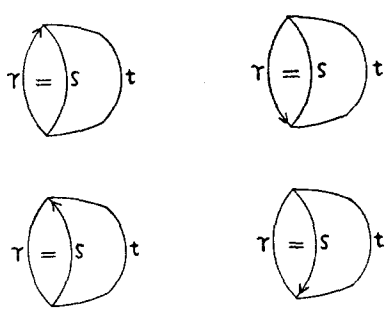
and it is therefore necessary to distinguish between the cases $r \neq t$ and $r=t$. Any dumbbell $(r,s,t)_d$ for which $r \neq t$ will be formed twice in the synthesis of $T_{n-r+1,r}$ in accordance with the scheme



and twice in the synthesis of $T_{n-t+1,t}$. If $r=t$ the dumbbell will be formed four times in the synthesis of $T_{n-r+1,r}$ in accordance with the scheme



The contribution to $\sum F_{r,n-r+1}$ is therefore always $4(r,s,t)_d$. Any star figure-eight $(r,s,t)_s$ will occur in the synthesis of $T_{n-r-s+1,r+s}$, $T_{n-r-t+1,r+t}$, $T_{n-s-t+1,s+t}$, if r, s, t are all different, and will be formed twice in each case to give a total contribution of $6(r,s,t)_s$. If any two of r, s, t are equal, $r=s$ say, then the constant will occur twice in $T_{n-r-s+1,r+s}$ and four times in $T_{n-r-t+1,r+t}$ in accordance with the scheme



Finally, if $r=s=t$, the constant will be formed six times in the synthesis of $T_{n-2r+1,2r}$.

We now have

$$c_{n+1}-2\sigma c_n+\sigma^2 c_{n-1} = 2np_n-2(n+1)p_{n+1}+8\sum_{n+1}(r,s,t)_d+8\sum_{n+1}p_r\cdot p_s +12\sum_{n+1}(r,s,t)_s \quad (5)$$

for $n>1$, the summations being taken over all the generalized figure-eights of order $n+1$ on the lattice.

The result (5), which we shall refer to as the "chain counting" theorem, was first discovered empirically in the following way. The successive chains were expressed in terms of the lattice constants p_{nx}, defined by Domb and Sykes,[7] for a general lattice. For convenience of reference, a table of the p_{nx} used here is given in Appendix I.

[7] C. Domb and M. F. Sykes, Phil. Mag. **2**, 733 (1957).

It was found that

$$\begin{aligned}
c_0&=1\\
c_1&=\sigma+1\\
c_2&=\sigma(\sigma+1)\\
c_3&=\sigma^2(\sigma+1)-6p_3\\
c_4&=\sigma^3(\sigma+1)-6p_3(2\sigma-1)-8p_4\\
c_5&=\sigma^4(\sigma+1)-6p_3(3\sigma^2-2\sigma)-8p_4(2\sigma-1)\\
&\qquad -10p_5+12p_{5a} \quad (6)\\
c_6&=\sigma^5(\sigma+1)-6p_3(4\sigma^3-3\sigma^2)-8p_4(3\sigma^2-2\sigma)\\
&\quad -10p_5(2\sigma-1)-12p_6+12p_{5a}(2\sigma)+12p_{6a}\\
&\qquad +12p_{6b}+8p_{6c}\\
c_7&=\sigma^6(\sigma+1)-6p_3(5\sigma^4-4\sigma^3)+8p_4(4\sigma^3-3\sigma^2)\\
&\quad -10p_5(3\sigma^2-2\sigma)-12p_6(2\sigma-1)-14p_7\\
&\quad +12p_{5a}(3\sigma^2)+12p_{6a}(2\sigma)+12p_{6b}(2\sigma)+8p_{6c}(2\sigma)\\
&\qquad +12p_{7a}+12p_{7b}+12p_{7f}+8p_{7d}+8p_{7e}.
\end{aligned}$$

On the right-hand side of (6) each p_{nx} occurs in c_{r+s} multiplied by a polynomial in σ, $\psi_{nx}{}^s(\sigma)$ say. It is easily seen that these polynomials satisfy the relation

$$\psi_{nx}{}^{s+2}=2\sigma\psi_{nx}{}^{s+1}-\sigma^2\psi_{nx}{}^s, \quad (7)$$

and it therefore only remains to discover how each lattice constant appears in (6) for the first time. An examination of the linear graphs corresponding to the lattice constants that occur in (6) together with those that occur in c_8, c_9, and c_{10} leads to the rules contained in (5).

The chain counting theorem enables the number of self-avoiding walks of n steps to be calculated recursively, the number of generalized figure-eights and polygons of order n being the only data required. It is of great practical use since for a given n there are very many fewer such structures than there are walks. With its aid the chain generating function $C(x)$ defined by Fisher and Sykes,[3]

$$C(x)=\sum_n c_n x^n, \quad c_0=1, \quad (8)$$

has been expanded on the simple quadratic lattice up to the term in x^{18} as

$$\begin{aligned}
C(x)=1&+4x+12x^2+36x^3+100x^4+284x^5+780x^6\\
&+2172x^7+5916x^8+16\,268x^9+44\,100x^{10}\\
&+120\,292x^{11}+324\,932x^{12}+881\,500x^{13}\\
&+2\,374\,444x^{14}+6\,416\,596x^{15}+17\,245\,332x^{16}\\
&+46\,466\,676x^{17}+124\,658\,732x^{18}+\cdots. \quad (9)
\end{aligned}$$

On this lattice the counting of the dumbbells required for the last two terms of (9) is laborious, and the author has been greatly assisted by Mr. B. J. Hiley in deriving and checking the data. For the three-dimensional simple cubic lattice, $C(x)$ has been expanded up to the term in x^{11}, and this series, together with those derived for the honeycomb, triangular, bcc, and fcc lattices, is given in Appendix II.

4. HIGH-TEMPERATURE ZERO-FIELD SUSCEPTIBILITY EXPANSION

Oguchi[1] has shown that the reduced susceptibility per spin of the Ising model $\chi(v)$, defined as $kT\chi_0/m^2$, may be expanded in powers of $v=\tanh K$,[8]

$$\chi(v)=\sum_r a_r v^r,$$

where $a_0=1$ and a_r is twice the term linear in N in the total number of ways of placing a graph of r lines on a lattice (of N sites) such that all but two of the vertices are the meet of an even number of lines. We may conveniently refer to such graphs as magnetic, the two vertices which are the meet of an odd number of lines being referred to as the magnetic vertices. The high-temperature counting problem presented by the susceptibility is that of evaluating the a_r for a given lattice. Some examples of magnetic configurations of order eight are given in Fig. 4. (The order of a configuration being the number of lines in the graph and hence the power of v to which it contributes. We shall refer to the number of lines that meet at a vertex as the order of that vertex.) Such configurations are numerous, and the counting of the large number of open types that occur (that is, configurations with at least one first-order vertex) rapidly becomes laborious and liable to error. Oguchi, who first derived series of this type, did not examine the counting problem in detail, although he remarked on its connection with the excluded volume problem. Domb and Sykes[7] give expressions for the first seven a_r in terms of lattice constants. These expressions are obtained by straightforward enumeration and reduction following the methods described by Domb.[4]

The coefficients (6) of the chain generating function possess the property

$$c_n-2\sigma c_{n-1}+\sigma^2 c_{n-2}=\text{linear sum lattice constants of order } n\ (n\geqslant 3). \quad (10)$$

It was remarked by Sykes[9] that the corresponding a_r of the susceptibility expansion of the Ising model appear to satisfy the property

$$a_n-2\sigma a_{n-1}+\sigma^2 a_{n-2}=\text{linear sum of lattice constants of order } n \text{ or less } (n\geqslant 3). \quad (11)$$

We have therefore sought to discover the general form of the right-hand side of (11) that would correspond to (5). We write

$$\chi(v)=(1-\sigma v)^{-2}[1-(\sigma-1)v-\sigma v^2+\sum_3^\infty d_r v^r], \quad (12)$$

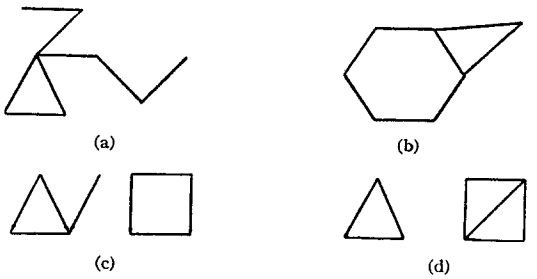


FIG. 4. Examples of eighth-order magnetic configurations: (a) connected open; (b) connected closed; (c) separated open; (d) separated closed.

the factor $(1-\sigma v)^{-2}$ corresponding to the left-hand side of (11), and the first five sums are found to be

$$\begin{aligned}
d_3&=-6p_3\\
d_4&=-8p_4\\
d_5&=6p_3-10p_5+8p_{5a}\\
d_6&=6p_3+8p_4-12p_6+28p_{5a}+8(p_{6a}+p_{6b}+p_{6c})\\
d_7&=10p_5-14p_7+36p_{5a}+16p_{6a}+30p_{6b}+16p_{6c}\\
&\quad+8(p_{7a}+p_{7b}+p_{7c}+p_{7d}+p_{7e}+p_{7f})+44p_{7g}.
\end{aligned} \quad (13)$$

There seems no obvious way of guessing the general form of the d_r in (13). The most irregular behavior is noticed for the more complicated no-field[10] lattice constants such as p_{7g}. These constants also occur in the expansion of the partition function in the absence of an applied field, and we therefore seek a combination of these two expansions to simplify (13). The presence of terms of the type $2sp_s$ suggests a differentiation of the term $p_s v^s$ with respect to v, and this corresponds to expanding the configurational energy. We therefore select the function

$$2vU(v)=\sum_r b_r v^r,$$

where $U(v)$ is the reduced energy $[U(0)=0,\ U(1)=q/2]$ for which

$$\begin{aligned}
b_0&=0\\
b_1&=0\\
b_2&=\sigma+1\\
b_3&=6p_3\\
b_4&=8p_4\\
b_5&=-6p_3+10p_5\\
b_6&=-6p_3-8p_4+12p_6-12p_{5a}\\
b_7&=-10p_5+14p_7-28p_{5a}-14p_{6b}-28p_{7g}.
\end{aligned} \quad (14)$$

We now form the quantity (b_s+d_s) for $s=3$ to $s=7$

[8] *Note.* Here χ_0 is the initial susceptibility per spin, k is Boltzmann's constant, m the moment of a single spin, $K=J/kT$, and J is the interaction energy between parallel spins. For details of the derivation of this result, reference should be made to the original paper of Oguchi and also to the review article by Domb.[4]

[9] M. F. Sykes, thesis, University of Oxford, 1956.

[10] *Note.* A no-field lattice constant is one all of whose vertices are even. They contribute to the partition function in the absence of an applied field (Domb[4]).

and obtain

$$\begin{aligned}
&b_3+d_3=0\\
&b_4+d_4=0\\
&b_5+d_5=8p_{5a}\\
&b_6+d_6=16p_{5a}+8(p_{6a}+p_{6b}+p_{6c})\\
&b_7+d_7=8p_{5a}+16(p_{6a}+p_{6b}+p_{6c})+8(p_{7a}+p_{7b}+p_{7c}\\
&\qquad\qquad+p_{7d}+p_{7e}+p_{7f})+16p_{7g}.
\end{aligned}\tag{15}$$

Equations (15) are remarkable in that all the polygons have canceled and the coefficients of the remaining lattice constants are all simple multiples of eight. Further, we notice that the coefficients g_r defined by

$$8\sum_r g_r v^r=(1+v)^{-2}\sum_s (b_s+d_s)v^s \tag{16}$$

will satisfy a recurrence relation of type (10) in place of (11).

We have now found empirically a rearrangement of the susceptibility expansion (12) which makes each new coefficient, up to $n=7$, depend on a function of the configurational energy and a linear sum of lattice constants (g_n) which satisfies the three conditions

(a) only lattice constants of order n occur in g_n;
(b) only no-field and magnetic lattice constants occur;
(c) every topologically possible magnetic lattice constant of order n appears with a positive nonzero coefficient. (17)

When the rearrangement is made for the eighth term for which

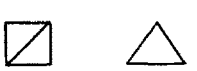
$$\begin{aligned}
d_8=&-16p_8+12p_6+8p_7-6p_3-28p_{5a}+56p_{6a}\\
&+24p_{6b}+8p_{6c}-48p_{6d}+32p_{7a}+32p_{7b}+32p_{7c}\\
&+16p_{7d}+16p_{7e}+16p_{7f}+8p_{7g}+8(p_{8a}+p_{8b}+p_{8c}\\
&+p_{8d}+p_{8e}+p_{8f}+p_{8g}+p_{8h}+p_{8j}+p_{8k}+p_{8l}+p_{8p}\\
&+6p_{8r}+6p_{8s}),
\end{aligned}\tag{18}$$

it is found that some constants of order less than eight remain in g_8 and that this linear sum also contains lattice constants with more than two odd vertices, for example, $96p_{6d}$ (tetrahedron).

Since the simplification already obtained is unlikely to be completely fortuitous, we now seek a modification of the conditions (17) which would enable the eighth term to be included. This can be achieved as follows. We now relax the condition that lattice constants are connected configurations. Thus we must regard configurations such as


symbol $[p_3,p_3]$

and (19)


symbol $[p_{5a},p_3]$

as lattice constants and denote the coefficient of N in the number of such configurations by $[p_3,p_3]$ and $[p_{5a},p_3]$, respectively. With this extended definition we can satisfy all the conditions (17) by making the substitution

$$\begin{aligned}
8[p_{5a},p_3]=8(&-p_{8l}-p_{8m}-p_{8q}-3p_{7g}\\
&-2p_{7c}-12p_{6d}-2p_{5a})
\end{aligned}\tag{20}$$

in (18). Then, on adding

$$\begin{aligned}
b_8=&+16p_8-12p_6-8p_4+6p_3+12p_{5a}-48p_{6a}-16p_{6b}\\
&-48p_{6d}-16p_{7a}-16p_{7b}-32p_{7c}-32p_{8r}-32p_{8s},
\end{aligned}\tag{21}$$

all the polygons cancel, and we obtain

$$\begin{aligned}
b_8+d_8=&8(p_{6a}+p_{6b}+p_{6c})+16(p_{7a}+p_{7b}+p_{7c}+p_{7d}\\
&+p_{7e}+p_{7f})+32p_{7g}+8(p_{8a}+p_{8b}+p_{8c}+p_{8d}\\
&+p_{8e}+p_{8f}+p_{8g}+p_{8h}+p_{8j}+p_{8k}+2p_{8l}+p_{8m}\\
&+p_{8p}+p_{8q}+2p_{8r}+2p_{8s}+[p_{5a},p_3]).
\end{aligned}\tag{22}$$

The right-hand side of (22) now follows the pattern of (15), and after application of the recurrence relation (16) the corresponding g_8 will satisfy the conditions (17).

5. SUSCEPTIBILITY COUNTING THEOREM

We can now state a hypothetical high-temperature counting theorem for the susceptibility expansion as follows. The expansion may be written

$$\begin{aligned}
\chi(v)=(1-\sigma v)^{-2}[&1-(\sigma-1)v+v^2-2vU(v)\\
&+8(1+v)^2\sum_r^{\infty} g_r v^r],
\end{aligned}\tag{23}$$

where g_r is a linear sum of lattice constants, including separated lattice constants, satisfying the conditions (17). We write this linear sum

$$g_r=\sum_{\text{all } x} w_{rx}p_{rx} \tag{24}$$

and call each w_{rx} the *counting weight* of the associated configuration.

To complete the enunciation of the theorem we require an expression for the counting weight of a lattice constant. In the chain counting theorem (5) the contribution of a lattice constant depends on its topology, the distinction between a dumbbell and a star being one of connectivity[11] that cannot be expressed in terms of the order of the vertices alone. From the nature of the Ising problem it seems intuitively unlikely that such a rule could obtain, and if rule there is, we should expect it to depend on the order of the vertices alone.

The counting weights of all the lattice constants of order eight or less are obtained by writing the first eight terms of the susceptibility expansion in the

[11] Because of this it seems likely that an exact solution of the excluded volume problem would be more difficult than an exact solution of the Ising problem in the presence of an applied field.

form (23). For the eighth term there are 61 topologically distinct magnetic configurations required by Oguchi's method. To obtain the general coefficient for higher order by direct enumeration and counting is laborious. We have therefore determined as many higher-order counting weights as possible by choosing particular lattices whose structure excludes many of the configurations that must be included in the general coefficient. By carrying through Oguchi's method all those ninth-order constants that can occur on a loose-packed lattice have been weighted. From an examination of the results obtained we postulate the following rules for the counting weight of a lattice constant.

(a) No-field lattice constants:

any number of second-order vertices and

1 fourth-order vertex	weight = 1	(25)
2 fourth-order vertices	weight = 2	
3 fourth-order vertices	weight = 3	
1 sixth-order vertex	weight = 3	

(b) Magnetic lattice constants[12]:

2 third-order magnetic vertices	weight = 1
1 third- and 1 fifth-order magnetic vertex	weight = 2

The direct proof of these rules for the most general case of a lattice of coordination number q along the lines of the corresponding long-chain counting theorem would seem to be very involved and we have not achieved it. For the particular case of $q=3$, however, a considerable simplification results and the proof although long has been carried through. It proceeds on the same lines as that of the chain counting theorem. In view of the complexity of a direct treatment of the general counting problem we shall not attempt to prove the theorem for $q>3$ but shall regard it as proved for $q=3$ and hypothetical for $q>3$.

The validity of the rules (a) and (b) has been tested by evaluating the counting weights of higher-order lattice constants. The special methods employed to do this together with an outline of the ways in which the rules were deduced is given in Appendix III. A further verification is afforded by the use of the exact susceptibilities of finite clusters of spins (some examples are given in Appendix IV) and also by a study of the susceptibility expansions of the honeycomb, triangular, and simple quadratic lattices. For the honeycomb lattice $q=3$, and for this case the susceptibility counting theorem has been established rigorously. From the susceptibility expansion of the honeycomb lattice we may derive that of the triangular lattice by transformation,[13] and this enables us to test the counting theorem for $q=6$. For the simple quadratic lattice the theorem can be tested for $q=4$ by deriving the susceptibility expansion by an independent method. The theorem can be used to extend the susceptibility expansions of three-dimensional lattices, but we shall not quote any new results here as the calculations have not yet been finally checked.

[12] We shall not quote any rules for magnetic lattice constants with two fifth-order vertices or with any magnetic vertex of order greater than five. They can be investigated by the methods of Appendixes III and IV.

6. SUSCEPTIBILITY EXPANSIONS OF THE HONEYCOMB AND TRIANGULAR LATTICES

The susceptibility expansions for the honeycomb and triangular lattices are conveniently considered together as they are closely related to one another. The precise form of this relationship has been given by Fisher.[13] If $\chi_H(w)$ denotes the reduced susceptibility of the honeycomb lattice and $\chi_T(v)$ denotes the reduced susceptibility of the triangular lattice, then

$$\chi_T(v)=\tfrac{1}{2}[\chi_H(w)+\chi_H(-w)] \quad \text{for} \quad w^2=v(1+v)/1+v^3. \tag{26}$$

Equation (26) relates the susceptibility of the triangular lattice to the mean of the ferromagnetic and antiferromagnetic susceptibilities of the honeycomb at a different temperature. For our present purpose we observe that from the high-temperature expansion for the susceptibility of the honeycomb lattice

$$\chi_H(w)=1+3w+6w^2+12w^3+24w^4+48w^5+90v^6+, \tag{27}$$

the corresponding series for the triangular lattice may be obtained by setting the odd coefficients equal to zero and substituting

$$w^2=v(1+v)/1+v^3=v+v^2-v^4+v^7+\cdots. \tag{28}$$

The counting theorem on the honeycomb as a result of the coordination number 3 and the rules (25) is extremely simple. The only possible no-field configurations are polygons or groups of separated polygons, and these all have zero counting weight. The only possible closed magnetic configurations fall into two classes:

(I) Dumbbells or dumbbells associated with one or more separated polygons.

(II) Figure-eight stars or figure-eight stars associated with one or more separated polygons.

Both these classes will have counting weight 1. The counting of these configurations on the honeycomb lattice is straightforward and does not become very laborious until $n=23$, while the direct method of Oguchi becomes involved after $n=13$.

As an example for the 19th term there are only eight cases to be considered and we quote these in Table I.

Proceeding in this way the first 24 g_r have been

[13] M. E. Fisher, Phys. Rev. **113**, 969 (1959).

TABLE I. Contributions to g_{19} on honeycomb lattice.

Class I	$(6,7,6)_d=69$	
	$(6,3,10)_d=42$	
	$(6,1,12)_d=9$	
	$[(6,1,6)_d,p_6]=-18$	
		Total $166\frac{1}{2}$
Class II	$(3,3,13)_s=6$	
	$(3,7,9)_s=6$	
	$(5,1,13)_s=39$	
	$(1,9,9)_s=13\frac{1}{2}$	

TABLE II. Contributions to g_9 and g_{10} on triangular lattice.

		g_9	g_{10}	wt
No-field:	one fourth-order vertex	108	−54	1
	two fourth-order vertices	48	261	2
	three fourth-order vertices	2	12	3
	one sixth-order vertex	2	6	3
Magnetic:	two third-order vertices	2547	11 787	1
	one fifth-order, one third-order vertex	54	252	2
	Total contribution:	2871	12 813	

evaluated. We find

$$\sum_{r=3}^{24} g_r v^r = \tfrac{3}{2}v^{11}+\tfrac{3}{2}v^{13}+6v^{14}+15v^{15}+12v^{16}+30v^{17}+67v^{18}+166\tfrac{1}{2}v^{19}+204v^{20}+421\tfrac{1}{2}v^{21}+1017v^{22}+1837\tfrac{1}{2}v^{23}+2613v^{24}. \quad (29)$$

The expansion (29) together with that for the energy of the honeycomb lattice, which is known from the work of Houtappel,[14] suffices to deduce the first 24 terms of the corresponding susceptibility expansion as

$$\chi_H(w)=1+3w+6w^2+12w^3+24w^4+48w^5+90w^6+168w^7+318w^8+600w^9+1098w^{10}+2004w^{11}+3696w^{12}+6792w^{13}+12\,270w^{14}+22\,140w^{15}+40\,224w^{16}+72\,888w^{17}+130\,650w^{18}+234\,012w^{19}+421\,176w^{20}+756\,624w^{21}+1\,348\,998w^{22}+2\,403\,840w^{23}+4\,299\,018w^{24}+\cdots. \quad (30)$$

From (30) and (26) we can derive the susceptibility expansion for the triangular lattice up to the term in in v^{12} as

$$\chi_T(v)=1+6v+30v^2+138v^3+606v^4+2586v^5+10\,818v^6+44\,574v^7+181\,542v^8+732\,678v^9+2\,935\,218v^{10}+11\,687\,202v^{11}+46\,296\,210v^{12}+\cdots. \quad (31)$$

From (31) the first 12 g_r for the triangular lattice have been deduced by manipulation into the form (23). The configurational energy of the triangular lattice is known from the work of Houtappel,[14] but as his paper contains a typographical error we quote the corrected expression in terms of the variable v:

$$-2vU(v)=\left[\frac{1-3v-3v^2+v^3}{(1-v)^3}\frac{2}{\pi}K(k)-1\right](1+v^2), \quad (32)$$

where $K(k)$ is the complete elliptic integral of the first kind and

$$k^2=16v^3(1-v+v^2)/(1-v)^6(1+v)^2.$$

[14] R. M. F. Houtappel, Physica **16**, 425 (1950).

From (32), we derive

$$2vU(v)=6v^2+12v^3+24v^4+48v^5+108v^6+276v^7+756v^8+2160v^9+6372v^{10}+19\,284v^{11}+59\,568v^{12}\cdots. \quad (33)$$

On using (33) and (31) in conjunction with (23), we obtain for the triangular lattice

$$\sum_{r=3}^{12} g_r v^r = 3v^5+21v^6+120v^7+615v^8+2871v^9+12\,813v^{10}+55\,410v^{11}+234\,393v^{12}. \quad (34)$$

In view of the complexity of the counting problem on the triangular lattice, the series (31) is most easily obtained by transformation of the honeycomb series (30). The validity of the hypothetical rules (25) for $q=6$ has been tested by deriving the terms up to v^{10} of (34) directly.

In the example given for the honeycomb lattice (g_{19}), the terms contributing have been grouped topologically. For the purpose of enumeration and counting this classification is convenient. For our present purpose, however, a topological description is redundant except in so far as it provides information about the vertex distribution. To verify the rules (25) for (34), it is sufficient to observe that all possible closed no-field and magnetic configurations of up to 10 lines on the triangular lattice fall into six groups summarized in Table II with their respective occurrences for $n=9$ and $n=10$. Each entry in Table II corresponds to a variety of topologies. For example, to obtain the number of 10th-order no-field configurations with one fourth-order vertex, we require (in the notation of Sec. 2)

$$\begin{aligned} &p_7\cdot p_3=540\\ &p_6\cdot p_4=276\\ &p_5\cdot p_5=108 \qquad \text{total } -54.\\ &[p_3\cdot p_3,\ p_4]=-312\\ &[p_3,\ p_3\cdot p_4]=-666 \end{aligned}$$

The fact that g_9 and g_{10} obtained in this way agree with those transformed from (30) provides a verification of the rules (25). The series (30) can be used

to evaluate the antiferromagnetic susceptibility of the triangular lattice over the whole temperature range $v=0$ to $v=-1$.[13] This application is reserved for a separate paper.

7. SUSCEPTIBILITY EXPANSION FOR THE SIMPLE QUADRATIC LATTICE

The first nine terms of the expansion for the simple quadratic lattice have been derived by Brooks and Domb[15] using a matrix method. They find

$$\chi(v)=1+4v+12v^2+36v^3+100v^4+276v^5+740v^6 +1972v^7+5172v^8+13\,492v^9+\cdots. \quad (35)$$

With the use of the counting theorem we have derived the six further terms:

$$+34\,876v^{10}+89\,764v^{11}+229\,628v^{12}+585\,508v^{13} +1\,486\,308v^{14}+3\,763\,460v^{15}+\cdots. \quad (36)$$

Since for the simple quadratic lattice $q=4$, all magnetic configurations will have two third-order vertices, and all no-field configurations will be made up of second- and fourth-order vertices. As a partial check on (36) we have derived the coefficients of v^{10} and v^{11} by an independent method. The configurational partition function for the simple quadratic lattice may be expanded at low temperatures[16] as a double series in the variables $\mu=\exp(-2mH/kT)$, $u=\exp(-4J/kT)$

$$\Lambda(\mu,u)=\sum_s f_s(u)\mu^s, \quad (37)$$

where $f_s(u)$ is a finite polynomial in u. The values of $f_1(u)$ to $f_8(u)$ obtained by Domb[16] and Brooks and Domb[15] are given by Domb and Sykes.[17] By enumeration and counting of low-temperature configurations, two further polynomials have been added to (37). The details of this derivation will be given in a separate paper, but we quote the result:

$$f_9(u)=u^6+72u^7+546u^8-1222u^9-18\,964u^{10} -694u^{11}+649\,535u^{12}-2\,932\,576u^{13} +6\,311\,938u^{14}-7\,804\,442u^{15}+5\,685\,542u^{16} -2\,278\,538u^{17}+388\,802u^{18}, \quad (38a)$$

$$f_{10}(u)=30u^7+462u^8+1230u^9-14\,444u^{10} -65\,862u^{11}+262\,160u^{12}+2\,228\,858u^{13} -16\,244\,768u^{14}+47\,256\,224u^{15} -78\,352\,726u^{16}+80\,010\,676u^{17} -50\,032\,548u^{18}+17\,649\,910u^{19} -2\,699\,202u^{20}. \quad (38b)$$

From (37) the corresponding high-temperature expansion

$$\Lambda(\mu,u)=\sum_r \frac{\phi_r(\mu)(1-u)^r}{(1+\mu)^{2r-1}}, \quad (39)$$

where the $\phi_r(\mu)$ are symmetric polynomials in μ, may be derived by manipulation.[16] The results (38) enable us to derive the first 11 polynomials $\phi_r(\mu)$, and following the method of Brooks and Domb[15] the susceptibility is obtained as a series in powers of $(1-u)$ which, after manipulation, yields (35) and the two extra terms $34\,876v^{10}+89\,764v^{11}$, confirming (36).

For a study of the ferromagnetic susceptibility of the simple quadratic lattice, the first nine terms of $\chi(v)$, (35), are adequate.[18] For the antiferromagnetic susceptibility the further terms (36) are required since the coefficients then alternate in sign and the extrapolation is a more delicate one. The antiferromagnetic susceptibility is to be discussed in a forthcoming paper.

8. CONCLUSIONS

A theorem has been derived that makes the exact enumeration of chains c_n on a lattice depend on a restricted class of closed graphs (generalized figure-eights), and this enables a substantial number of terms to be evaluated. A corresponding theorem has been developed empirically (and proved rigorously for the honeycomb lattice) for the susceptibility, and it is found that we may write

$$\chi(v)=(1-\sigma v)^{-2}[1-(\sigma-1)v+v^2-2vU(v) +8(1+v)^2\textstyle\sum_r g_r v^r], \quad (40)$$

where the g_r depend on the number of a restricted class of closed graphs. The enumeration problem of Oguchi has been transformed in such a way that only closed graphs with at most two odd vertices contribute.

The coefficients a_r are all positive and the series $\chi(v)$ converges up to the transition point for $J>0$. This occurs at the ferromagnetic Curie temperature T_c, and if v_f is the corresponding critical value of v, then $v_f=\tanh J/kT_c$. For negative interaction energies the series converges for $|v|\leqslant v_f$. The successive a_r form a fairly smooth sequence, but for the antiferromagnetic susceptibility the alternation of sign that corresponds to a negative interaction energy makes the problem of summation delicate. While we have derived (40) and the expansions given here with a view to investigating the antiferromagnetic susceptibility by extrapolation, we now observe that the susceptibility counting theorem admits of a more physical interpretation.

The result (40) contains an unknown function $G(v)$ defined by

$$G(v)=8(1+v)^2\textstyle\sum_r g_r v^r. \quad (41)$$

If we neglect $G(v)$, we obtain an approximation to the susceptibility, which we shall call the energetic suscep-

[15] J. E. Brooks and C. Domb, Proc. Roy. Soc. (London) **A207**, 343 (1951).
[16] C. Domb, Proc. Roy. Soc. (London) **A199**, 199 (1949).
[17] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A235**, 247 (1956); (a) *Note.* The two earlier papers[15,16] contain misprints.
[18] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A240**, 214 (1957).

tibility (χ_E), which for plane lattices whose energy is known may be evaluated over the entire temperature range $v=0$ to $v=-1$. For a two-dimensional loose-packed lattice such as the simple quadratic lattice, the energy in the region $|v|\simeq v_f$ behaves like[19]

$$a+b(T-T_c)\log|T-T_c|, \qquad (42)$$

where a and b are constants, and the energetic susceptibility will therefore also have a singularity of this type.[20] The conclusion that $\chi(v)$ will have a singularity of type (42) at $|v|=v_f$ could of course, be nullified by the behavior of $G(v)$. Sykes and Fisher[20] rejected this contingency on numerical grounds, and the conjecture that the antiferromagnetic susceptibility has a singularity analogous to that of the energy has subsequently been proved by Fisher[21] for the simple quadratic lattice. This gives one considerable confidence that our interpretation of (40) is correct and that the energy, which is determined by the first-order correlations between spins, plays a dominant role at temperatures above and in the neighborhood of the transition point. Further investigation shows that the function $G(v)$, which we shall call the residual correlation function, is essentially a low-temperature function important only in the region $v\simeq -1$ when, owing to the onset of complete (simple quadratic lattice) or partial (triangular lattice) order, the effect of higher-order correlations becomes larger. It is intended to make a more complete examination of this aspect of (40) in separate papers on the susceptibilities of the triangular and simple quadratic lattices.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge the constant encouragement and advice of Professor C. Domb. The author is also indebted to Dr. M. E. Fisher for stimulating discussions, to Dr. S. Katsura for helpful correspondence, and to B. J. Hiley for his assistance in deriving configurational data.

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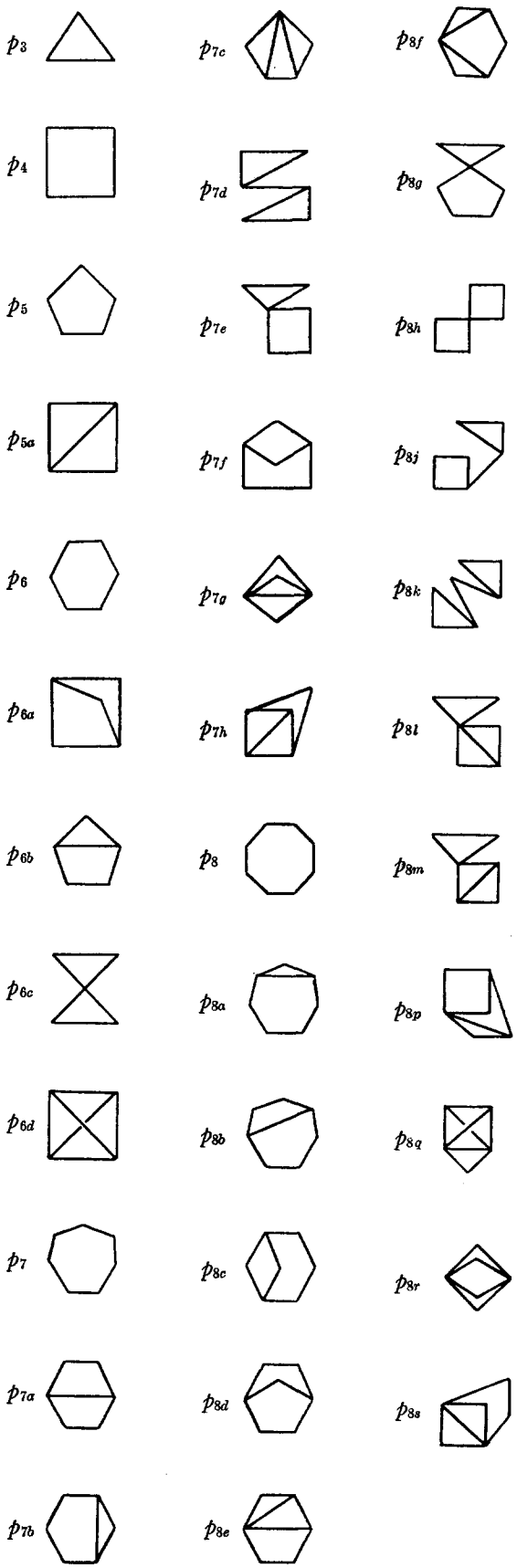
APPENDIX I. KEY TO THE LATTICE CONSTANTS USED IN THE TEXT

Following the notation of Domb and Sykes,[7] we associate each closed graph of n lines with a symbol p_{nx}, the suffix x differentiating between graphs of the same order but different topology. The numerical value of Np_{nx} for a given lattice of N sites is the number of distinct ways the graph p_{nx} can be placed on the lattice. Values of the p_{nx} for most simple lattices are given by Domb and Sykes[7] for $n\leqslant 7$ and for $n>7$ by Domb.[4]



[19] L. Onsager, Phys. Rev. **65**, 117 (1944).
[20] M. F. Sykes and M. E. Fisher, Phys. Rev. Letters **1**, 321 (1958).
[21] M. E. Fisher, Physica **25**, 521 (1959).

APPENDIX II. EXPANSIONS OF $C(x)$ NOT QUOTED IN THE TEXT

Honeycomb lattice:

$$C(x)=1+3x+6x^2+12x^3+24x^4+48x^5+90x^6+174x^7+336x^8+648x^9+1218x^{10}+2328x^{11}+4416x^{12}+8388x^{13}+15\,780x^{14}+29\,892x^{15}+56\,268x^{16}+106\,200x^{17}+199\,350x^{18}+375\,504x^{19}+704\,304x^{20}+1\,323\,996x^{21}+2\,479\,692x^{22}+4\,654\,464x^{23}+8\,710\,212x^{24}+\cdots.$$

Triangular lattice:

$$C(x)=1+6x+30x^2+138x^3+618x^4+2730x^5+11\,946x^6+51\,882x^7+224\,130x^8+964\,134x^9+4\,133\,166x^{10}+17\,668\,938x^{11}+\cdots.$$

Simple cubic lattice:

$$C(x)=1+6x+30x^2+150x^3+726x^4+3534x^5+16\,926x^6+81\,390x^7+387\,966x^8+1\,853\,886x^9+8\,809\,878x^{10}+41\,933\,286x^{11}+\cdots.$$

Body-centered cubic lattice:

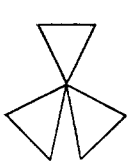
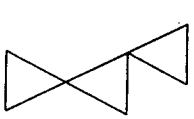
$$C(x)=1+8x+56x^2+392x^3+2648x^4+17\,960x^5+120\,056x^6+804\,824x^7+5\,351\,720x^8+35\,652\,680x^9+\cdots.$$

Face-centered cubic lattice:

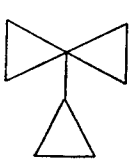
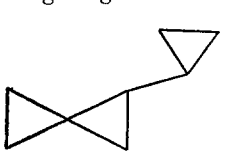
$$C(x)=1+12x+132x^2+1404x^3+14\,700x^4+152\,532x^5+1\,573\,716x^6+16\,172\,148x^7+165\,697\,044x^8+\cdots.$$

APPENDIX III. DETERMINATION OF COUNTING WEIGHTS

For eight lines there are 61 topologically distinct magnetic configurations required by Oguchi's method. To obtain the general expression for higher-order coefficients is laborious, and we therefore seek to deduce the counting weights of more complex graphs by using special structures. For example, if we suppose that the lattice is a triangular cactus, made by joining together a fixed number of triangles at each point, then for the ninth term there are only 18 possible magnetic configurations, and by counting these we deduce the counting weights of

 $=3$ and of  $=2$. (A1)

By enumerating all the 10th-order magnetic terms we deduce the further counting weights

 $=2$ and  $=1$. (A2)

By examining the five special terms in the 12th-order coefficient we deduce that the counting weight of four triangles meeting at a point is 6. The argument may be generalized to show that the counting weight of r triangles meeting at a point is $\frac{1}{2}r(r-1)$.

If r triangles meet at a point the corresponding vertex is of order $2r=\theta$, say. But $\frac{1}{2}r(r-1)=\theta(\theta-2)/8$, and this quantity vanishes for all the other vertices of such a structure. We therefore postulate as a generalization that the counting weight of any no-field configuration will always be $\sum\theta(\theta-2)/8$, where θ is the order of each vertex and the summation is taken over all the vertices. This rule will be found to be valid for all the results obtained so far. From it we may deduce that the counting weight of the pentagon with all bonds

should be 5. This lattice constant will occur in the 10th coefficient, but it is difficult to evaluate its contribution directly. That the result is correct will be shown in the Appendix IV.

APPENDIX IV. USE OF FINITE CLUSTERS TO CHECK AND DERIVE COUNTING WEIGHTS

A study of the exact partition functions of finite clusters provides a method of checking the counting weights so far derived and can be employed to derive new ones. As an illustration of the method we shall examine a cluster of five spins all connected to one another (close-packed cluster), which we denote by $CP(5)$. The partition function in the absence of an applied field and the susceptibility of this cluster are easily derived by elementary methods, and we find

$$(\text{p.f.})=32(1-v^2)^{-5}(1+10v^3+15v^4+12v^5+15v^6+10v^7+v^{10}) \quad \text{(B1)}$$

and

$$\chi(v)=(1+6v^2+6v^3+6v^4+v^6)/(1-4v+10v^2-10v^3+10v^4-4v^5+v^6). \quad \text{(B2)}$$

By manipulation of (B1) and (B2), we may obtain $\chi(v)$ in the form (23) and deduce that for this cluster

$$\sum_{r=3}^{\infty} g_r v^r=6v^5+17v^6+16v^7-54v^8-258v^9-486v^{10}+\cdots. \quad \text{(B3)}$$

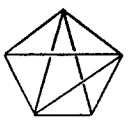
It is evident that if any rules of the type postulated in (25) are to hold, we must assume that if the counting weight of $[p_{nx},p_{my}]$ is denoted by $[w_{nx},w_{my}]$; then

$$[w_{nx},w_{my}]=w_{nx}+w_{my}. \quad \text{(B4)}$$

An examination of $CP(5)$ now shows that the coefficient of v^9 must be composed of four separated lattice constants

$$[p_{6a}, p_3] = -20$$
$$[p_{6b}, p_3] = -120$$
$$[p_{6c}, p_3] = -30$$
$$[p_{5a}, p_4] = -90$$

all of weight 1 and contributing -260 to g_9, and one new constant

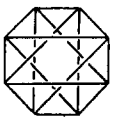


of value 2 per site. If the coefficient of v^9 is to be that in (B3), the counting weight of this constant must be taken as unity.

In a like manner, for the coefficient of v^{10} there are six separated configurations with a total contribution of -487 and one connected configuration, the cluster itself

of value $\frac{1}{5}$. If the coefficient of v^{10} is to be that in (B3), we require a contribution of $+1$, and we deduce that the counting weight of the pentagon with all bonds is 5. This was originally predicted (Appendix III) by the result (A3).

The rules (25) have been further verified by using the exact partition functions and susceptibilities of a close-packed cluster of seven spins and the octahedron as well as for a number of loose-packed clusters such as

 and  .

Use of Series Expansions for the Ising Model Susceptibility and Excluded Volume Problem

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The present paper discusses the problem of making the most effective use of the coefficients of series expansions for the Ising model and excluded volume problem in estimating critical behavior. It is shown that after initial irregularities the coefficients appear to settle down to a smooth asymptotic behavior. Alternative methods of analysis are considered for the provision of a steady series of approximations to the critical point. Numerical conclusions are drawn for particular lattices for which additional terms have recently become available.

1. INTRODUCTION

IN a previous paper[1] it has been shown how, by the use of certain configuration counting theorems, substantial numbers of terms of series expansions can be derived for the susceptibility of the Ising model and for the excluded volume problem. It is the purpose of the present paper to undertake numerical analysis of the coefficients in such expansions, and to show that after initial irregularities they appear to settle down to a smooth asymptotic behavior which can be accurately estimated.

The extrapolation of numerical data must usually proceed with care and caution. Fortunately, however, in the problems which we shall discuss some exact information is already available regarding the asymptotic form of the coefficients. Thus for the Ising model in two or three dimensions it is known from the work of Yang and Lee[2] that a spontaneous magnetization exists below T_c and hence that the initial susceptibility is infinite at the Curie point. Therefore, if we write this susceptibility in the form

$$X_0=\sum a_n w^n \qquad w=\tanh(J/kT), \tag{1}$$

we know that $a_n \sim \phi(n)/w_c{}^n$, where

$$\lim_{n\to\infty} [\phi(n)]^{1/n}=1 \tag{2}$$

(w_c corresponds to the Curie point).

It is natural to try to fit $\phi(n)$ by an expression of the form

$$\phi(n)\sim An^g. \tag{3}$$

To assess whether this estimation is in reasonable accord with the numerical data, it is convenient to plot a_n/a_{n-1} as a function of $1/n$. If expression (3) is valid,

$$a_n/a_{n-1}\simeq(1/w_c)(1+g/n), \tag{4}$$

and hence we should obtain a straight line whose intersection with $1/n=0$ determines w_c, and whose slope determines g.

The said method was used by Domb and Sykes[3] who found that the numerical data then available fitted well to a formula of type (3). For two-dimensional lattices w_c is known exactly, and they were able to conjecture that g was equal to $\frac{3}{4}$, and hence that the singularity in the susceptibility at the Curie point was of the form $(1-T_c/T)^{-7/4}$.

This conjecture subsequently received rigorous support from the work of Fisher[4] who determined the nature of the singularity by summing the correlations over all distances. The method was also applied by Domb and Sykes to three-dimensional models.

The theorems of the previous paper enable several new terms to be added to the data used by Domb and Sykes, and the numerical analysis of the present paper enables the Curie point to be estimated with increased accuracy for three-dimensional models; the conjecture that for such models g is equal to $\frac{1}{4}$ is further substantiated and the corresponding singularity in the susceptibility is of the form $(1-T_c/T)^{-5/4}$.[5]

In regard to the excluded volume problem, if c_n is the number of nonintersecting chains of n units, it is known rigorously from the work of Hammersley[6] that

$$c_n\sim\phi(n)\mu^n, \tag{5}$$

where $\phi(n)$ satisfies the relation (2). An investigation determining μ and g from a relation of type (3) was undertaken by Fisher and Sykes.[7] Now that more numerical data are available, a more comprehensive investigation can be undertaken.

The numerical method can also be applied to estimate the asymptotic form of the number of simple closed polygons p_n on a crystal lattice, and to investigate the relation between the asymptotic forms of c_n and p_n.

[1] M. F. Sykes, J. Math. Phys. **2**, 52 (1961), preceding paper.
[2] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952).
[3] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A240**, 214 (1957).
[4] M. E. Fisher, Physica **25**, 521 (1959).
[5] It may be noted that the comparison of coefficients for different values of spin given by Domb and Sykes[3] gave a strong indication that the asymptotic forms of the susceptibility given here for two- and three-dimensional lattices are valid for all values of spin.
[6] J. M. Hammersley, Proc. Cambridge Phil. Soc. **53**, 642 (1957).
[7] M. E. Fisher and M. F. Sykes, Phys. Rev. **114**, 45 (1959).

A more detailed treatment of these applications to the excluded volume problem will be given elsewhere,[8] but we shall make a comparison of the behavior of the chains c_n with that of the closely related a_n in Eq. (1).

We give in an Appendix the susceptibility expansions for the simple cubic, body-centered cubic, and face-centered cubic lattices in the form of Eq. (1). The other data employed in this paper are already presented elsewhere.[1,8]

2. SUSCEPTIBILITY EXPANSIONS FOR THE ISING MODEL

High-temperature expansions for the initial susceptibility of the Ising model have been examined by Domb and Sykes[3] who employed the development in inverse powers of the temperature. Asymptotically this is equivalent to the form (1) and it is computationally more convenient to employ the variable $w=\tanh(J/kT)$ for higher terms. That the available data fit well to a formula of type (4) is illustrated in Fig. 1, where we plot a_n/qa_{n-1} against $1/n$ for the fcc and triangular lattices. (It is convenient for the purpose of comparison to take out the coordination number q as a factor, since this makes the maximum energy the same for both lattices.) It will be seen that for $n>3$ the plot is remarkably linear and for the triangular lattice the known exact limit is clearly indicated.[9] Loose-packed lattices, such as the simple quadratic lattice, show a marked oscillation between "odd" and "even" ratios and, to estimate the limiting intercept at $n=\infty$, Domb and Sykes used the linear

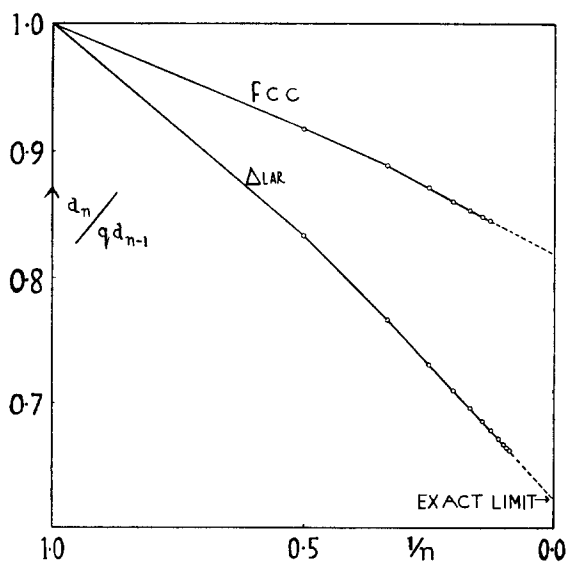

FIG. 1. Ising model. Successive ratios in the susceptibility expansions of the triangular and fcc lattices as functions of $1/n$.

[8] B. J. Hiley and M. F. Sykes (unpublished).

[9] The formula (4) is exact, if a_n is the nth coefficient in the expansion of $(1-w)^{-g-1}$. The close fit, even for relatively small n, shows that such a function provides a good approximation for the susceptibility.

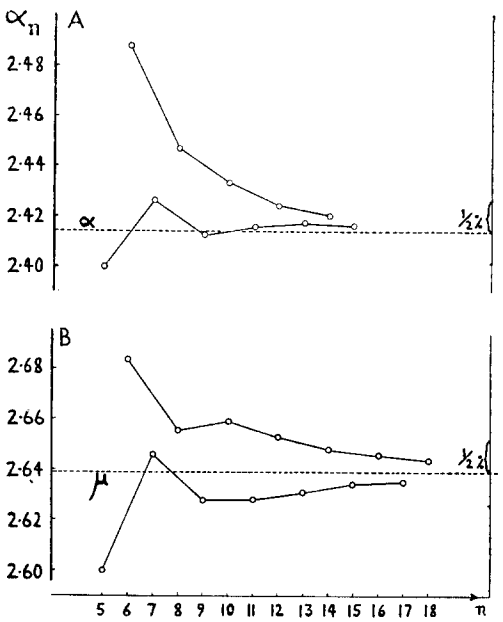

FIG. 2. Estimates for the critical parameters of the simple quadratic lattice by the method of linear projection as functions of n. (A) Ising problem. $\alpha_n=\frac{1}{2}[na_n/a_{n-1}-(n-2)a_{n-2}/a_{n-3}]$. Exact limit $(\alpha)=2.4142$. (B) Excluded volume problem. $\alpha_n=\frac{1}{2}[nc_n/c_{n-1}-(n-2)c_{n-2}/c_{n-3}]$. Extrapolated limit $(\mu)=2.6395$.

projections α_n of alternate pairs of points

$$\alpha_n=\tfrac{1}{2}[na_n/a_{n-1}-(n-2)a_{n-2}/a_{n-3}]. \qquad (6)$$

While the distinction between odd and even ratios is not strictly necessary for close-packed lattices, the successive α_n still give smoother estimates for the critical temperature than the linear projections of adjacent points. In Fig. 2(A) we plot the values of α_n for the simple quadratic lattice against n from $n=5$ to $n=15$. With nine terms at their disposal, Domb and Sykes concluded that while the successive estimates were close to the true value [marked by the dashed line α in Fig. 2(A)], their behavior was somewhat irregular and made accurate extrapolation difficult. It can be seen from Fig. 2(A) that a more regular behavior develops for values of $n>9$.

However, to make the most effective use of the new data for the provision of accurate estimates of the critical point, the method of linear projections, which depends on pairs of ratios, is not particularly suitable, since it magnifies small irregularities in the data. We have instead used the function

$$\beta_n=na_n/qa_{n-1}(n+g) \qquad (7)$$

against $1/n$, where g is first estimated by the method of Fig. 1. By virtue of expression (4), β_n tends to $1/qw_c$ as $n\rightarrow\infty$, and it is a function of one ratio only. The additional factor $(n+g)$ has the effect of straightening out the limit horizontally. Even if the estimate of g is in error, the limit of β_n is still $1/qw_c$, but the approach to this limit is not quite horizontal.

In Fig. 3(A) the successive β_n are plotted against $1/n$ for the simple quadratic lattice with $g=\frac{3}{4}$. The behavior of the β_n is smoother than that of the α_n and the last seven values are all within $\frac{1}{2}\%$ of the known exact limit (0.60355) which we shall denote by β_a. In Fig. 3(A) we have marked the value $\frac{1}{2}\%$ above this, which we denote by β_a^+, and below this, which we denote by β_a^-. The estimates improve steadily with increasing n.

We have added two more coefficients to the series for the simple cubic lattice and in Fig. 3(B) and Fig. 3(C) we plot the corresponding β_n for the simple cubic and bcc lattices with $g=\frac{1}{4}$. It will be seen that the behavior is more regular and remarkably similar for these two lattices and we would suggest that the conjecture $g=\frac{1}{4}$ is exact. We consider that the critical values for these two lattices which we denote by β_b and β_c, respectively, probably lie between the pairs of curves in Figs. 3(B) and 3(C), and we estimate

$$1/qw_c=0.7640\pm0.0010 \quad \text{for the simple cubic,}$$
$$\text{and} \qquad (8)$$
$$1/qw_c=0.8004\pm0.0010 \quad \text{for the bcc.}$$

As remarked in the Introduction, care is needed in performing extrapolations of this kind and the limits of error quoted in Eqs. (8) are based on the assumption

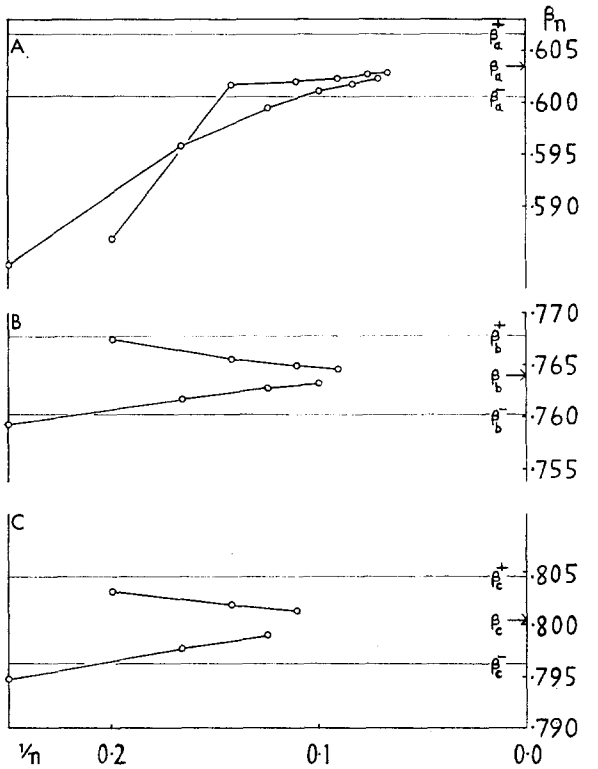

FIG. 3. Ising model. Estimation of critical temperatures by extrapolation of β_n. $\beta_n=na_n/qa_{n-1}(n+g)$. (A) Simple quadratic lattice; $g=\frac{3}{4}$. Exact limit $\beta_a=0.6036$. $\beta_a^+=1.005\beta_a$, $\beta_a^-=0.995\beta_a$. (B) Simple cubic lattice; $g=\frac{1}{4}$. Extrapolated limit $\beta_b=0.7640$. $\beta_b^+=1.005\beta_b$, $\beta_b^-=0.995\beta_b$. (C) Body-centered cubic lattice; $g=\frac{1}{4}$. Extrapolated limit $\beta_c=0.8004$. $\beta_c^+=1.005\beta_c$, $\beta_c^-=0.995\beta_c$.

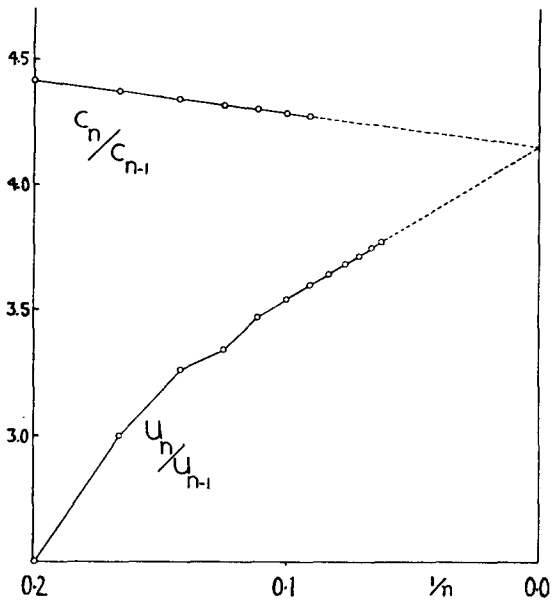

FIG. 4. Excluded volume problem. Successive ratios in the expansions of $C(x)$ and $U(x)$ for the triangular lattice as functions of $1/n$.

that the observed trends persist for large n, an assumption supported by Fig. 3(A). We have marked in Figs. 3(B) and 3(C) the values $\frac{1}{2}\%$ above (β_b^+, β_c^+) and below (β_b^-, β_c^-) the estimated limits, and it would appear most unlikely that the true critical values lie outside this range. It would seem that the method provides an improving sequence of estimates for the critical temperature of a three-dimensional lattice. In a similar manner we estimate that for the fcc lattice

$$1/qw_c=0.8192\pm0.0010. \qquad (9)$$

3. EXCLUDED VOLUME PROBLEM

In the excluded volume problem series expansions closely related to the high-temperature Ising series arise.[10] Two examples of these are the expansions of the generating functions $C(x)$ and $U(x)$ for non-self-intersecting walks and simple closed polygons, respectively. If c_n is the number of non-self-intersecting walks of n steps and u_n the number of non-self-intersecting returns to the origin after n steps on a lattice, then

$$C(x)=\sum_n c_n x^n, \quad c_0=1$$
$$U(x)=\sum_n u_n x^n, \quad u_0=1. \qquad (10)$$

In Fig. 4 we plot the successive ratios c_n/c_{n-1} and u_n/u_{n-1} for the triangular lattice against $1/n$. For $C(x)$ we have used the first 11 coefficients given by

[10] For a precise statement of the underlying enumeration problems the reader is referred to the paper by Sykes[1] and a recent review article by Domb.[11] See also H. N. V. Temperley, Phys. Rev. **103**, 1 (1956), and Fisher and Sykes.[7]

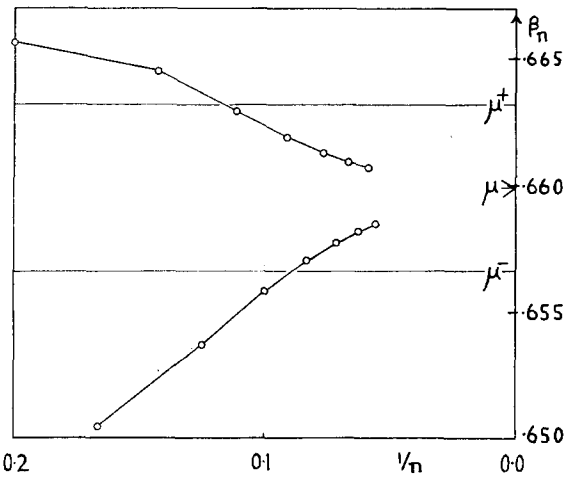

FIG. 5. Excluded volume problem. Estimation of the critical parameter μ for the simple quadratic lattice by extrapolation of β_n. Extrapolated limit $\mu=2.6390$. $\mu^+=1.005\mu$, $\mu^-=0.995\mu$.

Sykes and for $U(x)$ the coefficients up to x^{16} have been derived by using a method based on the existence of a dual lattice (Domb).[11] It will be seen that there is a striking similarity in the behavior of the ratios c_n/c_{n-1} and the ratios a_n/qa_{n-1} of the corresponding susceptibility series for this lattice (Fig. 1). It is to be inferred from Fig. 4 that the two sequences c_n/c_{n-1} and u_n/u_{n-1} have a common limit, which we shall denote by μ, and that[7]

$$c_n \sim n^g \mu^n$$
$$u_n \sim n^h \mu^n, \tag{11}$$

the values of g and h being determined by the slopes of the two lines in Fig. 4. It will be noticed that while the expansion of $C(x)$ is well behaved for small values of $n(\sim 5)$, the corresponding expansion of $U(x)$ does not settle down to a smooth behavior until $n>10$. This is not surprising in view of the comparative rarity of polygonal returns to the origin for small values of n.

To investigate whether there is any closer analogy in behavior between the coefficients c_n of $C(x)$ and a_n of $X_0(w)$, we have calculated for the simple quadratic lattice the α_n corresponding to Eq. (6) for the function $C(x)$; that is,

$$\alpha_n=\tfrac{1}{2}[nc_n/c_{n-1}-(n-2)c_{n-2}/c_{n-3}]. \tag{12}$$

The coefficients are available up to x^{18} and the result is given in Fig. 2(B). The value of μ (2.6395 ± 0.0010) marked in the figure is that of Fisher and Sykes[7]; it is in very good agreement with that of Wall.[12] Wall's estimate (2.6395 ± 0.0015) is based on a Monte Carlo method in which very long walks are sampled (of the order of $n=800$). The very close agreement of these two estimates, obtained by quite independent methods, provides confirmation of the proposed limit and also of the asymptotic behavior [see Eq. (11)] on which the estimate from $C(x)$ is based.

It will be seen from Fig. 2(B) that a smooth behavior for the α_n sets in at about $n=9$ as it does in the corresponding Ising series [Fig. 2(A)]. It is, therefore, to be hoped that conclusions drawn from these series will prove as reliable as those that have been drawn for the Ising problem. As in the Ising problem it is found that the corresponding β_n are somewhat more regular, and Fisher and Sykes[7] have suggested that for a plane lattice, g in expression (11) is exactly $\frac{1}{3}$.

We have plotted in Fig. 5 the corresponding β_n with this value for the simple quadratic lattice, that is

$$\beta_n=nc_n/qc_{n-1}(n+\tfrac{1}{3}). \tag{13}$$

(It is convenient to take out a factor q in this problem also so as to facilitate comparison between different lattices.) The symmetry of Fig. 2(B) is reflected in Fig. 5 where we have marked the values $\frac{1}{2}\%$ above and below the estimated limit by μ^+ and μ^-. We shall not examine these data in any further detail, since our primary object is to draw attention to the close similarity in the behavior of series expansions of the type $X(w)$ and $C(x)$. The excluded volume problem is to be the subject of a separate paper,[8] and we shall only remark that further numerical analysis of the data in Fig. 5 enables a more precise estimate of μ to be made as

$$\mu=2.6390\pm0.0005. \tag{14}$$

It is clear from Fig. 4 that a good estimate of the asymptotic behavior of the function $U(x)$ can now be made, and this will be undertaken in the paper referred to previously. In some respects, we may think of the series $C(x)$ and $U(x)$ as *high-temperature expansions*, for while x is only a dummy variable, there is a close analogy with the behavior of high-temperature expansions for the Ising model in powers of the high-temperature counting variable w. In general these high-temperature expansions are characterized by smooth behavior of their coefficients, enabling the radius of convergence and asymptotic behavior to be estimated with some confidence.

4. CONCLUSIONS

We have shown by an examination of the available data that the coefficients in some series expansions that arise in the theory of the Ising model and the excluded volume problem behave smoothly and provide a reasonable basis for extrapolations. We have been guided by the known exact behavior for two-dimensional Ising models and have made estimates for the critical temperatures of some three-dimensional lattices. We collect these results in a table together with those for the excluded volume problem parameter μ taken from Fisher and Sykes.[7]

It can be seen from Table I that while the critical values of both $1/qw$ and μ/q for plane lattices or

[11] C. Domb, Advances in Phys. (to be published).
[12] F. T. Wall and J. J. Erpenbeck, J. Chem. Phys. **30**, 634 (1959).

TABLE I. Critical values for the Ising model and excluded volume problem.

		sq	Δ lar	sc	bcc	fcc
Ising model	$1/qw_c$	0.6036	0.6220	0.7640	0.8004	0.8192
Excluded volume problem	μ/q	0.6599	0.6920	0.7816	0.8175	0.8375

three-dimensional lattices are close together there is a wider separation between two- and three-dimensional lattices. It would seem that dimensionality plays a dominant role in these problems and this observation extends also to the asymptotic behavior of the coefficients. The further evidence we have examined enables us to suggest with increased confidence that while the susceptibility of a plane Ising lattice has a singularity at the Curie point of the form $(1-T_c/T)^{-7/4}$, for a three-dimensional lattice the corresponding singularity will be of the form $(1-T_c/T)^{-5/4}$.

For the excluded volume problem it has been suggested by Fisher and Sykes that $c_n \sim n^{1/3}\mu^n$ for a two-dimensional lattice, the index $\frac{1}{3}$ being indicated for the simple quadratic, triangular, and honeycomb lattices. For three-dimensional lattices the data are not so extensive but the index (0.17 ± 0.03) is approximately the same for the simple cubic, bcc, and fcc lattices. In this problem too it would seem that dimensionality is of primary importance in determining asymptotic behavior.

ACKNOWLEDGMENTS

We are indebted to Dr. M. E. Fisher for many stimulating discussions. One of us (M.F.S.) would like to express his gratitude to the University of London for the award of an I.C.I. fellowship.

APPENDIX

Susceptibility expansions for three-dimensional lattices. We give the expansion in powers of w of the reduced susceptibility as defined in the previous paper.[1]

Simple cubic lattice.

$$1+6w+30w^2+150w^3+726w^4+3510w^5+16\,710w^6+79\,494w^7+375\,174w^8+1\,769\,686w^9+8\,306\,670w^{10}+38\,972\,214w^{11}.$$

Body-centered cubic lattice.

$$1+8w+56w^2+392w^3+2648w^4+17\,864w^5+118\,760w^6+789\,032w^7+5\,201\,048w^8+34\,268\,104w^9.$$

Face-centered cubic lattice.

$$1+12w+132w^2+1404w^3+14\,652w^4+151\,116w^5+1\,546\,332w^6+15\,734\,460w^7+159\,425\,580w^8.$$

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On the General Theory of the Approach to Equilibrium. II. Interacting Particles

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The general method described in a recent paper by Prigogine and Henin [J. Math. Phys. **1**, 349 (1960), hereafter referred to as I] is applied to a system of interacting particles. A full use is made of the diagram technique due to Prigogine and Balescu. The distribution function is Fourier analyzed and each Fourier coefficient is decomposed into two parts: one (ρ') whose evolution results from scattering processes and which obeys a diagonal differential equation; the second one (ρ''), whose evolution is due to direct mechanical interactions which build the correlation described by the Fourier coefficient. The ρ'' can be expressed in terms of functions ρ' corresponding to lower correlations. We study first the velocity distribution function. Only scattering processes contribute to the evolution of this function. The equations obtained ensure evolution of this function to the correct equilibrium value at any order in the concentration C and the coupling constant λ. We then study the asymptotic behavior of the Fourier coefficients which describe correlations among the particles. The part ρ' of these coefficients corresponding to scattering processes vanishes for large time. In other words, scattering processes play a fundamental role in the establishment of the correct velocity distribution function, but once this is achieved they become ineffective. The correct equilibrium correlations, which in equilibrium theory are described in terms of cluster diagrams, are built by direct mechanical interactions among the particles involved in the correlation. We give a detailed proof up to order C^2. The extension to higher orders does not introduce any new feature.

1. INTRODUCTION

IN a recent paper,[1] I. Prigogine and one of us (F.H.) have shown that it is possible to study formally the problem of the evolution in time of a system of interacting normal modes up to an arbitrary finite order in the coupling constant λ. This was made possible through a systematic use of the diagram technique developed in preceding papers.[1-3]

The diagrams so introduced describe the dynamics of the correlations which exist among the normal modes. Their asymptotic behavior for a very large number of degrees of freedom and long time is suprisingly simple. There are two main classes of diagrams which contribute asymptotically: first of all, diagrams corresponding to a succession of independent scattering events, and secondly diagrams which describe the building up of the correlations. The Fourier components which describe those correlations can also be divided into two parts. Through this decomposition, the behavior of the system for long times becomes very clear. In the case of interacting normal modes, it has been possible to show that up to order λ^2, the system reaches the correct equilibrium distribution. The mathematical complexity of the operators involved made it difficult to give a proof valid at an arbitrary order. This was mainly due to the action dependence of the interaction energy, which leads to a "renormalization" of the frequencies.

From this point of view, the situation is much simpler in the case of interacting particles with a potential energy which is only a function of the coordinates. At equilibrium the velocity distribution function is simply a function of the unperturbed Hamiltonian. All correlations which exist in the system are also quite simple functions. This made it possible to establish a general H theorem, valid to any arbitrary order $C^m\lambda^n$ (m at least finite), where C is the concentration.

First of all, we establish the evolution equations for the velocity distribution function and the correlations in Fourier space. This is done by exactly the same method as for interacting normal modes. A minor difference between the two problems is however the diagram technique. We deal here with particles which have an individuality, whereas in the case of interacting normal modes we deal with excitations with no individuality. The differences appear in the fact that connected diagrams actually now play an important role. In fact, those diagrams determine the irreversible behavior of the system. Indeed, they are the only diagrams which contribute to the evolution of reduced distribution functions of a finite number of degrees of freedom, which are the only functions for which an irreversible behavior might be expected. This problem has been treated in two papers by Prigogine and Balescu.[2,3] All details concerning the Fourier expansion of the distribution function, the initial conditions and the basic diagrams can be found in those papers; however, one remark has to be made concerning the time dependence of general diagrams. In footnote references 2 and 3, all calculations were done in the interaction representation; however, some features are then not very clear. In fact, when the usual representation is used, the time dependence of the general diagrams becomes much simpler. General theorems concerning this point will be derived in the Appendix. By taking into account these theorems, one can again, as in the case of interacting normal modes, decompose any Fourier component describing a given correlation

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[1] I. Prigogine and F. Henin, J. Math. Phys. **1**, 349 (1960), hereafter referred to as I.
[2] I. Prigogine and R. Balescu, Physica **25**, 281 (1959).
[3] I. Prigogine and R. Balescu, Physica **25**, 302 (1959).

into two parts: one $\rho'_{(\gamma)}$ which contains the effect of the scattering of the particles, the other $\rho''_{(\gamma)}$ which contains the effect of the direct mechanical interactions between the particles involved in the correlation. The functions $\rho'_{(\gamma)}$ obey quite simple diagonal differential equations whereas the functions $\rho''_{(\gamma)}$ can be expressed in terms of operators acting on the $\rho'_{(\gamma)}$ describing lower correlations.

As in the case of interacting normal modes, we take the coupling constant λ as parameter in order to derive these equations. This amounts to a classification of the diagrams according to the number of vertices involved. Although in the case of interacting normal modes this was the only expansion parameter, in the case of interacting particles we have another one, the concentration C. Very often, this is in fact the expansion parameter which should be used (strong forces). This, however, can easily be done by a mere regrouping of the terms involved in the equations obtained by expansion with respect to λ.

Then, instead of classifying the diagrams with respect to their number of vertices whatever the number of particles involved, one classifies them with respect to the number of particles whatever the number of vertices. This is actually a very interesting feature. Indeed, the behavior of the system, whatever parameter one wishes to take, can be inferred from a study of the diagrams which appear in the equations from either point of view: number of vertices and number of particles. This is in fact very easy to do. The general results are the following:

The velocity distribution function becomes for long times a function of the unperturbed energy as required by the general theory of equilibrium.

The part $\rho'_{(\gamma)}$ of the correlations vanishes for such time; and then the $\rho''_{(\gamma)}$ are entirely determined by the velocity distribution function.

In other words, the correct equilibrium correlations are built from a state without correlations by direct mechanical interactions of the particles involved in the correlation. Scattering effects play a role only in the establishment of the required velocity distribution function.

2. FOURIER ANALYSIS OF THE DISTRIBUTION FUNCTION

The Hamiltonian of the system is of the form

$$H=H_0+\lambda V$$
$$=\sum_{i=1}^{N}\mathbf{p}_i^2/2m+\lambda\sum_{i<j}V_{ij}(|\mathbf{x}_i-\mathbf{x}_j|). \quad (2.1)$$

The Liouville operator corresponding to this Hamiltonian is

$$L=L_0+\lambda\delta L$$
$$=\sum_i \mathbf{p}_i\cdot\frac{\partial}{\partial\mathbf{x}_i}-\lambda\sum_{i<j}\frac{\partial V_{ij}}{\partial\mathbf{x}_i}\cdot\mathbf{D}_{ij}, \quad (2.2)$$

where

$$\mathbf{D}_{ij}=\partial/\partial\mathbf{p}_i-\partial/\partial\mathbf{p}_j. \quad (2.3)$$

The distribution function $\rho(\{\mathbf{x}\}\{\mathbf{p}\}t)$ can be expanded in terms of the eigenfunctions of the unperturbed Liouville operator L_0 (for more details see footnote reference 2):

$$\rho(\{\mathbf{x}\}\{\mathbf{p}\}t)$$
$$=(8\pi^3\Omega)^{-N}\{\rho_0+\Omega^{-1}\sum_{\mathbf{k}}{}'\sum_j\rho_{\mathbf{k}}{}^j\exp[i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{v}_jt)]$$
$$+\Omega^{-1}\sum_{\mathbf{k}}{}'\sum_{j<l}\rho_{\mathbf{k}}{}^{jl}\exp[i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_l-\mathbf{v}_jt-\mathbf{v}_lt)]$$
$$+\Omega^{-2}\sum_{\mathbf{k}+\mathbf{k}'\neq0}{}'\sum_{\mathbf{k}'}{}'\sum_{j<l}\rho_{\mathbf{k}}{}^j{}_{\mathbf{k}'}{}^l$$
$$\times\exp[i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{v}_jt)+i\mathbf{k}'\cdot(\mathbf{x}_l-\mathbf{v}_lt)]+\cdots\}, \quad (2.4)$$

where we have ordered the various terms according to the number of nonvanishing wave vectors (the dash in the summations over wave vectors means that $\mathbf{k}=\mathbf{0}$ has to be excluded). As in footnote reference 2, we make the assumptions that the various Fourier coefficients do not depend explicitly on N or Ω in the asymptotic limit ($N\to\infty$, $\Omega\to\infty$ in such a way that N/Ω remains finite). The factor $(8\pi^3\Omega)^{-N}$ in front of (2.4) ensures normalization of the distribution function to unity. The other Ω^n factors (where n is the number of independent wave vectors in the corresponding coefficients, i.e., the number of nonvanishing wave vectors minus the number of relations of the form $\mathbf{k}_1+\mathbf{k}_2+\cdots=\mathbf{0}$ which exist among them) ensure that already at the initial time one can define extensive and intensive properties of the system in the thermodynamical sense.

The physical meaning of the Fourier coefficient ρ_0 plays a special role. This coefficient is just the velocity distribution function. All the other Fourier coefficients give us information about the spatial distribution, i.e., about the correlations which may exist between the particles, and the spatial inhomogeneities. More precisely, any Fourier coefficient such as $\rho_{\mathbf{k}1,\cdots,\mathbf{k}n}{}^{m1,\cdots,mn}$ with $\sum_{i=1}^n\mathbf{k}_i$ describes a correlation between n particles; whereas the same coefficient for which the sum of the wave vectors is nonvanishing is related to spatial inhomogeneities in the system.

A general Fourier coefficient can describe several correlations and contain several inhomogeneity factors. For instance, the Fourier coefficient

$$\rho_{\mathbf{k}1,\mathbf{k}2,\mathbf{k}3,\mathbf{k}4,\mathbf{k}5,\mathbf{k}6}{}^{m1,m2,m3,m4,m5,m6}$$
$$\text{with}\quad \mathbf{k}1+\mathbf{k}2+\mathbf{k}3=\mathbf{0},\quad \mathbf{k}4+\mathbf{k}5=\mathbf{0},\quad \mathbf{k}6\neq\mathbf{0}, \quad (2.5)$$

describes a triple correlation between particles $m1$, $m2$, $m3$, a double correlation between particles $m4$ and $m5$, and contains an inhomogeneity factor related to particle $m6$.

It is not necessary to study the behavior of such general coefficients. It can be shown that they can be factored into products of coefficients describing simply each of the correlations and inhomogeneity factors

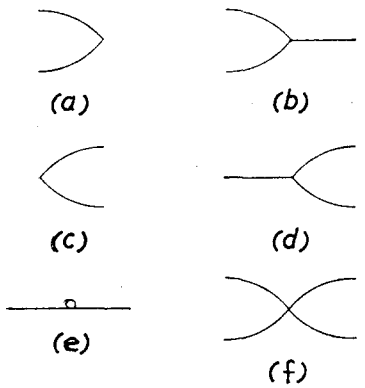


FIG. 1. Basic diagram. (a), (c): Creation (destruction) of a correlation; (b), (d): Increase (decrease) of the number of particles in a correlation; (e): Exchange of particles; (f): Propagation of correlation.

(for more details about this, see footnote reference 4). On introducing (2.4) in the Liouville equation for the distribution function, one obtains the evolution equation for those Fourier components:

$$\Omega^{-r}\partial\rho_{\mathbf{k}\alpha,\cdots\mathbf{k}\nu}{}^{\nu}/\partial t$$
$$=\lambda\Omega^{-1}\sum_{m<n}\exp[i(\mathbf{k}_\alpha\mathbf{v}_\alpha+\cdots+\mathbf{k}_\nu\mathbf{v}_\nu)t]$$
$$\times\{\langle\mathbf{k}_\alpha\cdots\mathbf{k}_\nu|\delta L_{mn}|\mathbf{0}\rangle\rho_0+\Omega^{-1}\sum_j$$
$$\times\sum_{\mathbf{k}j'}\langle\mathbf{k}_\alpha\cdots\mathbf{k}_\nu|\delta L_{mn}|\mathbf{k}_j'\rangle\exp(-i\mathbf{k}_j'\mathbf{v}_j t)\rho_{\mathbf{k}j',j}$$
$$+\Omega^{-2}\sum_{j<s}\sum_{\substack{\mathbf{k}_j',\mathbf{k}_s'\\ \mathbf{k}_j'+\mathbf{k}_s'\neq 0}}\langle\mathbf{k}_\alpha\cdots\mathbf{k}_\nu|\delta L_{mn}|\mathbf{k}_j'\mathbf{k}_s'\rangle$$
$$\times\exp[-i(\mathbf{k}_j'\mathbf{v}_j t+\mathbf{k}_s'\mathbf{v}_s t)]\rho_{\mathbf{k}j',\mathbf{k}s'}{}^{s}$$
$$+\Omega^{-1}\sum_{j<s}\sum_{\mathbf{k}j'}\langle\mathbf{k}_\alpha\cdots\mathbf{k}_\nu|\delta L_{mn}|\mathbf{k}_j',\mathbf{k}_s'=-\mathbf{k}_j'\rangle$$
$$\times\exp[-i\mathbf{k}_j'\cdot(\mathbf{v}_j-\mathbf{v}_s)t]\rho_{\mathbf{k}j',j}{}^{s}+\cdots\}, \quad (2.6)$$

where r represents the number of independent wave vectors in $\rho_{\mathbf{k}\alpha,\cdots\mathbf{k}\nu}{}^{\nu}$. The matrix elements in the rhs of (2.6) are given by

$$\langle\mathbf{k}_\alpha\cdots\mathbf{k}_\nu|\delta L_{mn}|\mathbf{k}_j'\cdots\mathbf{k}_s'\rangle$$
$$=(8\pi^3\Omega)^{-N}\int(d\mathbf{x})^N\exp[-i(\mathbf{k}_\alpha\mathbf{x}_\alpha+\cdots+\mathbf{k}_\nu\mathbf{x}_\nu)]$$
$$\times(\partial V_{mn}/\partial\mathbf{x}_m)\cdot\mathbf{D}_{mn}\exp[i(\mathbf{k}_j'\mathbf{x}_j+\cdots+\mathbf{k}_s'\mathbf{x}_s)]. \quad (2.7)$$

They represent a transition from the state $\{\mathbf{k}'\}$ to the state $\{\mathbf{k}\}$ due to an interaction between molecules m and n. They vanish unless all wave vectors $\mathbf{k}=\mathbf{k}'$, except $\mathbf{k}_m\neq\mathbf{k}_m'$, $\mathbf{k}_n\neq\mathbf{k}_n'$ with however the following conservation law:

$$\mathbf{k}_m'+\mathbf{k}_n'=\mathbf{k}_m+\mathbf{k}_n. \quad (2.8)$$

Because of these properties of the matrix elements of δL the set of equations (2.6) can be decomposed into independent subsets of equations. In each of these subsets, we have only Fourier coefficients with the same value of the total wave vector. For instance, for homogeneous systems, all Fourier coefficients are zero except those describing correlations among the particles (total wave vector vanishing). As those coefficients form an independent subset, if the system is initially homogeneous, it will remain so in the course of time.

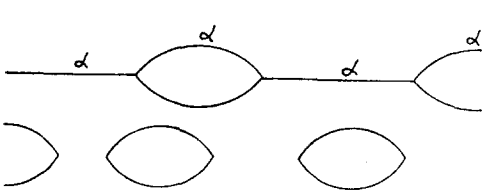


FIG. 2. Example of disconnected diagram (four disconnected parts); particle α propagates through the whole diagram.

[4] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience Publishers, Inc., New York, to be published).

3. HOMOGENEOUS SYSTEMS—FORMAL SOLUTION OF (2.6)—INITIAL CONDITIONS

Equations (2.6) can be formally solved by iteration. Any term of this formal solution is a product of matrix elements of δL times the initial value of a Fourier component and contains integrals over the time oscillating exponentials associated with those matrix elements. We wish to study the behavior of the system for large times t. For times t much larger than the duration of a collision, asymptotic integrations may be performed and any term of the formal solution of (2.6) becomes proportional to some power of λ and some power of t. In fact, any contribution is proportional to $\lambda^r(\lambda^2 t)^m$.

As is the study of interacting normal modes, we wish to keep all contributions up to a given, finite value of r. The easiest way to find the values of r and m corresponding to a given contribution is to make use of a diagram technique. This technique has been explained in footnote references 2 and 3. It consists mainly of associating a line to each nonvanishing wave vector. In this way one obtains a very simple picture of the dynamics of correlations as expressed by the evolution equations. The diagrams corresponding to the most general term in the formal solution of (2.6) can be classified according to quite general topological properties. Their time behavior is a direct consequence of their structure as we shall see in Sec. 4.

To specify completely the λ dependence of the various contributions, we have to choose a given class of initial conditions. We shall take the same initial conditions as in footnote reference 2 (for discussion see Sec. 12), namely,

$$\rho_{(\gamma)}(0)=O(\lambda^\gamma), \quad (3.1)$$

where

$$\rho_{(\gamma)}(0)=\rho_{\mathbf{k}1,\mathbf{k}2,\cdots\mathbf{k}(\gamma+1)}{}^{m1,m2,\cdots m(\gamma+1)}\quad\sum_{i=1}^{\gamma+1}\mathbf{k}i=\mathbf{0} \quad (3.2)$$

describes a correlation between $(\gamma+1)$ particles.

4. DIAGRAM—TIME DEPENDENCE

There are six basic types of vertices which have been introduced in footnote reference 2 (see Fig. 1). On

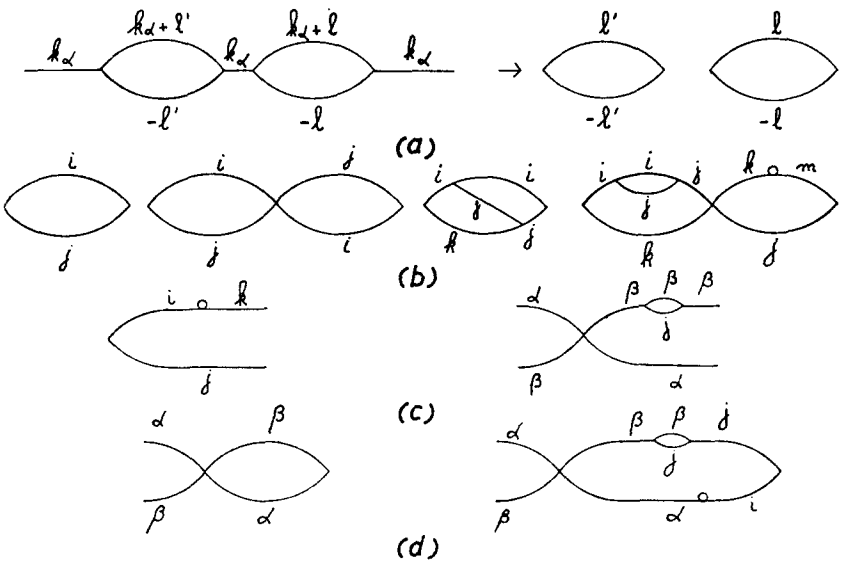


FIG. 3. Examples of connected basic structures: (a) a connected part and its basic structure; (b) diagonal connected basic structure; (c) destruction connected basic structure; (d) creation connected basic structure.

combining these basic vertices, we obtain various types of diagrams which we intend to classify according to their topological structure. Let us first decompose a given diagram into its disconnected parts (or semiconnected parts[2]), defined, as usual, in such a way that no propagation line connects any two vertices belonging to different disconnected parts (see Fig. 2).

Among these disconnected parts, some may have a line corresponding to the same particle α propagating through the whole diagram from 0 to t; because we want to describe such a propagation exactly, we shall not make any asymptotic integration on the wave vector describing this motion, but only on the wave vector associated with the interactions (see Appendix). As we want to maintain a close relationship between a given diagram and its asymptotic time dependence, we define the "basic structure" of a disconnected part as the diagram obtained by "subtracting" the line $\mathbf{k}_\alpha \mathbf{v}_\alpha$ (if any) in the given disconnected part. Let us notice that a connected diagram may have a disconnected basic structure [Fig. 3 (a)]. We may get the following possible connected basic structures:

(a) *Diagonal connected basic structure:* a diagram in which the initial and final states are the "vacuum" ($\{\mathbf{k}_i\}=\{0\}$) without any intermediate state with $\{\mathbf{k}_i\}=\{0\}$.

(b) *Creation connected basic structure:* a diagram which begins with the vacuum and ends with a final state $\{\mathbf{k}_i\}\neq\{0\}$.

(c) *Destruction connected basic structure:* a diagram of any kind in which the initial state differs from the vacuum. There are two kinds: those in which the final state is the vacuum and those in which the final state represents correlations.

We now generalize our definitions to any diagram, made up of many disconnected parts:

(a) *Diagonal fragment:* any combination of diagonal diagrams which is such that no intermediate states have $\{\mathbf{k}_i\}=\{0\}$.

(b) *Creation fragment:* any combination of creation and diagonal diagrams such that no intermediate states correspond to the vacuum.

(c) *Destruction fragment:* any combination of destruction and diagonal diagrams such that no intermediate states correspond to the vacuum. Examples are given in Fig. 4. Moreover, we shall often use the notation shown in Fig. 5, where (a), (b), and (c) represent, respectively, the sum of all diagonal, creation, and

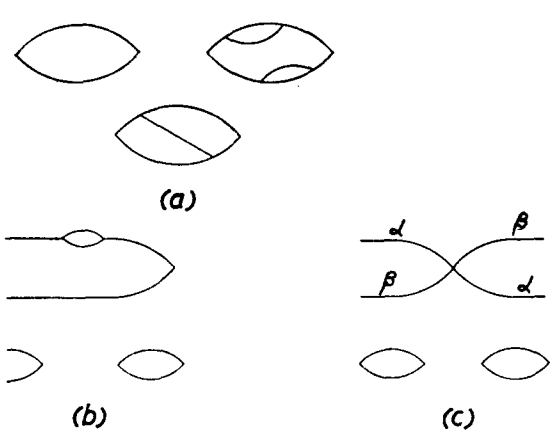


FIG. 4. Examples of fragments: (a) diagonal, (b) creation, (c) destruction.

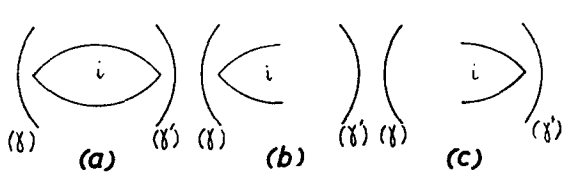


FIG. 5.

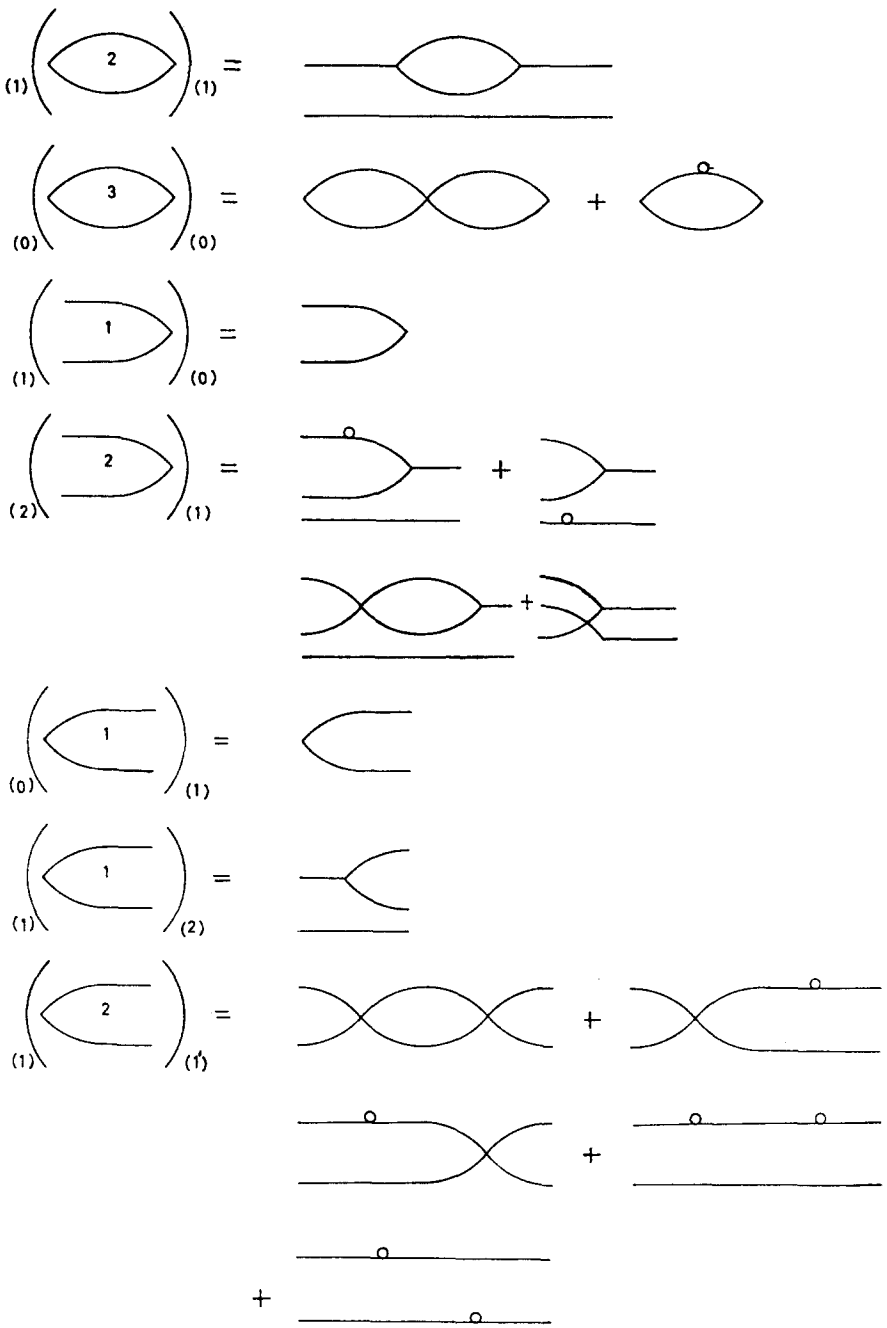


FIG. 6.

destruction fragments with i vertices which allow a transition from a state γ to a state γ'. Examples are given in Fig. 6.

In the following we shall not explicitly state that the terms "diagonal fragment," "creation fragment," and "destruction fragment" always refer to the basic structure of the given diagram; however, this will always be assumed. With these three basic types of diagrams, we can construct two general classes of diagrams. Any diagram in the formal solution of (2.6) will be met in one of these two classes. First, we have *reducible diagrams*, i.e., diagrams which can be decomposed into the following regions:

creation fragment | diagonal region | destruction fragment,

where the diagonal region is a succession of diagonal fragments. Particular cases are the diagonal diagrams, destruction diagrams, creation diagrams.[1]

In the second class, we have the *irreducible diagrams*, i.e., diagrams which cannot be decomposed into the

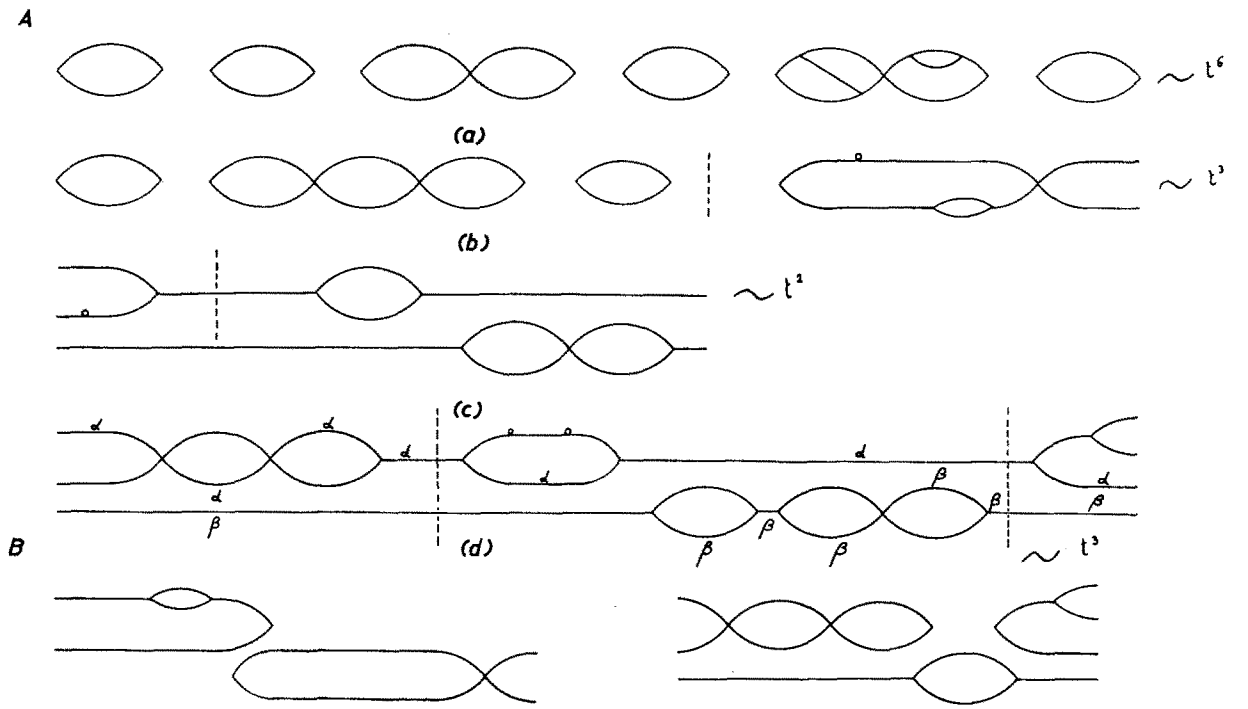


FIG. 7. (A) Reducible diagrams: (a) diagonal diagram, (b) destruction diagram, (c) creation diagram, (d) reducible creation-destruction diagrams. (B) Irreducible diagrams.

characteristic regions already described. They all contain a creation *and* a destruction fragment which cannot be separated. Examples of general diagrams are given in Fig. 7. The asymptotic contributions of these diagrams are derived in the Appendix. The theorems of footnote reference 1 are valid here also:

Theorem I. Any reducible diagram has an asymptotic contribution proportional to t^m, where m is the number of diagonal fragments in the diagonal region of the diagram.

Theorem II. Any irreducible diagram has a vanishing asymptotic contribution.

5. ASYMPTOTIC CONTRIBUTIONS TO THE FOURIER COMPONENTS

By taking into account the foregoing theorems, we see that we have only to consider the reducible diagrams. As in footnote reference 1, we shall subdivide them into two classes:

(1) Diagrams which contain *no* creation fragment, i.e., diagonal and destruction diagrams.

(2) Diagrams which contain a creation fragment, i.e., creation and reducible creation-destruction diagrams. We shall decompose the Fourier coefficients into two parts:

$$\exp[-i\sum_{j=1}^{\gamma+1}\mathbf{k}_j\mathbf{v}_j t]\rho_{(\gamma)}(t) = \exp[-i\sum_{j=1}^{\gamma+1}\mathbf{k}_j\mathbf{v}_j t]\rho'_{(\gamma)}(t)+\rho''_{(\gamma)}(t), \quad (5.1)$$

where $\rho'_{(\gamma)}(t)$ is made from all the contributions of the first class and will obey a diagonal equation (Sec. 6) whereas $\rho''_{(\gamma)}(t)$ is made from all the contributions of the second class and will be expressed in terms of the functions $\rho'_{(\gamma)}(t)$ (Sec. 7).

The physical meaning of this decomposition is the same as in footnote reference 1: the evolution of the functions $\rho'_{(\gamma)}(t)$ is due to scattering of the particles whereas the functions $\rho''_{(\gamma)}(t)$ depend on the direct mechanical interactions between the particles which build the correlation (γ).

On taking into account the initial conditions (3.1), one can expand the functions $\rho'_{(\gamma)}(t)$ in the following way:

$$\rho'_{(\gamma)}(t)=\lambda^\gamma\{\rho'_{(\gamma)}{}^{(0)}(t)+\lambda\rho'_{(\gamma)}{}^{(1)}(t)+\lambda^2\rho'_{(\gamma)}{}^{(2)}(t)+\cdots\}, \quad (5.2)$$

where the functions $\rho'_{(\gamma)}{}^{(r)}(t)$ contain all diagonal and destruction diagrams with asymptotic contribution proportional to $\lambda^r(\lambda^2 t)^m$, m arbitrary integer $\geqslant 0$. Equation (5.2) is, however, not a true expansion in power series of λ, because the initial values of the Fourier components may contain higher-order terms with respect to λ than those given in (3.1) and because the product $\lambda^2 t$ is itself λ dependent. In the same way, one can write

$$\rho''_{(\gamma)}(t)=\lambda^\gamma\{\rho''_{(\gamma)}{}^{(0)}(t)+\lambda\rho''_{(\gamma)}{}^{(1)}(t)+\lambda^2\rho''_{(\gamma)}{}^{(2)}(t)+\cdots\}, \quad \gamma\geqslant 1, \quad (5.3)$$

$$\rho''_{(0)}(t)=0, \quad (5.4)$$

where (5.4) expresses the fact that no creation fragments ever contribute to the evolution of $\rho_{(0)}$. Again $\rho''_{(\gamma)}{}^{(r)}(t)$ contains all creation and reducible creation-destruction diagrams with asymptotic contribution proportional to $\lambda^r(\lambda^2 t)^m$, m arbitrary $\geqslant 0$.

6. EVOLUTION EQUATIONS FOR THE FUNCTIONS $\rho'_{(\gamma)}{}^{(r)}(t)$

We shall prove that these functions obey the following equation:

$$\partial\rho'^{(r)}_{(\gamma)}/\partial t = \lambda^2 \sum_{i=0}^{r} \underset{(\gamma)}{\overset{(i+2)}{\bigcirc}}_{(\gamma)} \rho'^{(r-i)}_{(\gamma)}(t). \tag{6.1}$$

Let us first consider some simple examples. At order λ^0, we have just to consider the lowest order contributions to the velocity distribution function $\rho_0{}^{(0)}(t)$. The only diagrams which are asymptotically proportional to $(\lambda^2 t)^m$ are diagonal diagrams made of a succession of m cycles (see theorem I). Therefore we have

$$\rho'^{(0)}_0(t) = \rho_{0(0)} + \sum_{a=1}^{\infty} \left(\bigcirc\!\!\!\!2\right)^a \rho_{0(0)}$$

$$= \rho_{0(0)} + \lambda^2 \left(\bigcirc\!\!\!\!2\right) \int_0^t dt_1\, \rho_0^{(0)}(t_1). \tag{6.2}$$

By derivation with respect to time, one obtains the usual master equation for weakly coupled systems which is a particular case of (6.1) for $r=0$ and $\gamma=0$. At order λ, we have two new equations to take into account: one for the next-order velocity distribution function $\rho'_{(0)}{}^{(1)}(t)$ and another one for the lowest-order contribution to the Fourier component describing binary correlations $\rho'_{(1)}{}^{(0)}(t)$. Here again we have only diagonal diagrams. In the case of the velocity distribution we must include a diagonal fragment with three vertices among the cycles; whereas in the case of $\rho'_{(1)}{}^{(0)}(t)$ the extra λ factor comes from the initial conditions. We obtain for $\rho'_{(0)}{}^{(1)}(t)$

$$\rho'^{(1)}_{(0)}(t) = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^p \bigcirc\!\!\!\!3 \left(\bigcirc\!\!\!\!2\right)^q \rho_{0(0)}$$

$$= \lambda^2 \bigcirc\!\!\!\!3 \int_0^t dt_1 \sum_{q=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^q \rho_{0(0)}$$

$$+ \lambda^2 \bigcirc\!\!\!\!2 \int_0^t dt_1 \sum_{p=1}^{\infty}\sum_{q=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^{p-1} \bigcirc\!\!\!\!3$$

$$\times \left(\bigcirc\!\!\!\!2\right)^q \rho_{0(0)}$$

$$= \lambda^2 \bigcirc\!\!\!\!3 \int_0^t dt_1\, \rho_0^{(0)}(t_1) + \lambda^2 \bigcirc\!\!\!\!2 \int_0^t dt_1 \rho_0^{(1)}(t_1). \tag{6.3}$$

In the second step we have separated the contributions corresponding to $p=0$ and $p\neq 0$ and have written explicitly the first diagonal fragment at the left. All contributions at the right of the integral $\int_0^t dt_1$ have to be evaluated asymptotically up to time t_1.

The equation for $\rho'_{(1)}{}^{(0)}(t)$ is exactly the same as (6.2), with the only difference that the cycles are now on two lines corresponding to the existence of the binary correlation

$$\rho'^{(0)}_{(1)}(t) = \rho_{(1)(0)} + \sum_{a=1}^{\infty} \left\{ \underset{(1)}{\left(\bigcirc\!\!\!\!2\right)_{(1)}} \right\}^a \rho_{(1)(0)}$$

$$= \rho_{(1)(0)} + \underset{(1)}{\left(\bigcirc\!\!\!\!2\right)_{(1)}} \int_0^t dt_1\, \rho'^{(0)}_{(1)}(t_1). \tag{6.4}$$

At order λ^2, we have three new equations: for $\rho'_{(0)}{}^{(2)}(t)$, $\rho'_{(1)}{}^{(1)}(t)$ and $\rho'_{(2)}{}^{(0)}(t)$. In the case of $\rho'_{(0)}{}^{(2)}(t)$, the diagonal diagrams must be of order λ^2. This means that in addition to cycles, we must consider either two diagonal fragments with three vertices or one fragment with four vertices. Moreover, we can have destruction diagrams with one destruction transition [Fig. 1(c)] starting from a binary correlation:

$$\rho'^{(2)}_{(0)}(t) = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\sum_{m=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^p \bigcirc\!\!\!\!3 \left(\bigcirc\!\!\!\!2\right)^q$$

$$\times \bigcirc\!\!\!\!3 \left(\bigcirc\!\!\!\!2\right)^m \rho_{0(0)}$$

$$+ \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^p \bigcirc\!\!\!\!4 \left(\bigcirc\!\!\!\!2\right)^q \rho_{0(0)}$$

$$+ \sum_{p=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^p \subset \rho_{(1)(0)}. \tag{6.5}$$

If we consider separately the terms with $p=0$ and $p\neq 0$, we obtain the equation

$$\rho'^{(2)}_{(0)}(t) = \subset \rho_{(1)(0)} + \bigcirc\!\!\!\!4 \int_0^t dt_1 \left\{ \sum_{q=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^q \rho_{0(0)} \right\}$$

$$+ \bigcirc\!\!\!\!3 \int_0^t dt_1 \left\{ \sum_{q=0}^{\infty}\sum_{m=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^q \bigcirc\!\!\!\!3 \left(\bigcirc\!\!\!\!2\right)^m \rho_{0(0)} \right\}$$

$$+ \bigcirc\!\!\!\!2 \int_0^t dt_1 \left\{ \sum_{p=1}^{\infty}\sum_{q=0}^{\infty}\sum_{m=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^{p-1} \bigcirc\!\!\!\!3 \left(\bigcirc\!\!\!\!2\right)^q \right.$$

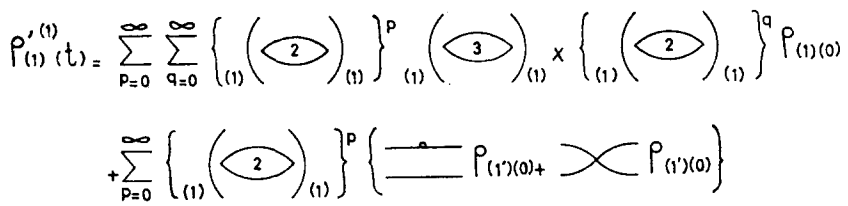
$$\times \bigcirc\!\!\!\!3 \left(\bigcirc\!\!\!\!2\right)^m \rho_{0(0)} + \sum_{p=1}^{\infty}\sum_{q=0}^{\infty} \left(\bigcirc\!\!\!\!2\right)^{p-1}$$

$$\left. \times \bigcirc\!\!\!\!4 \left(\bigcirc\!\!\!\!2\right)^q \rho_{0(0)} + \sum_{p=1}^{\infty} \left(\bigcirc\!\!\!\!2\right)^{p-1} \subset \rho_{(1)(0)} \right\}$$

$$= \subset \rho_{(1)(0)} + \bigcirc\!\!\!\!4 \int_0^t dt_1\, \rho_0^{(0)}(t_1) + \bigcirc\!\!\!\!3 \int_0^t dt_1 \rho_0^{(1)}(t_1)$$

$$+ \bigcirc\!\!\!\!2 \int_0^t dt_1\, \rho_0^{(2)}(t_1), \tag{6.6}$$

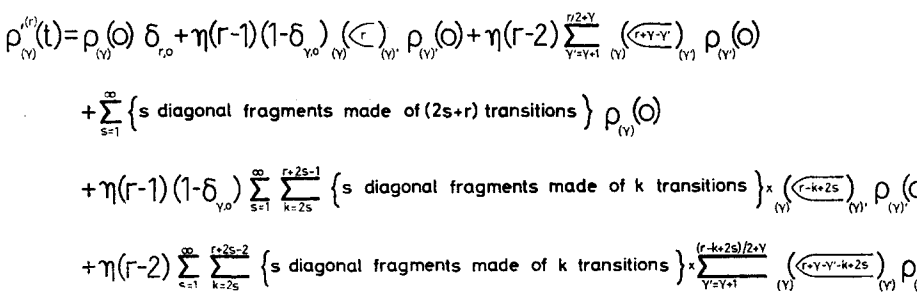
where we have taken account of (6.2), (6.3), and (6.5). As the first term on the rhs of (6.6) is a constant, by derivation with respect to time we obtain (6.1). The diagonal contributions to $\rho'_{(1)}{}^{(1)}(t)$ are the same as those to $\rho'_{(0)}{}^{(1)}(t)$, two lines being added to the cycles; however, in this case, at the left we can also have vertices of the type (e) or (f) of Fig. 1. Therefore, we have the equation



(6.7)

where (1′) means that the correlation in the initial state is different from that in the final state either by one of the particles involved or by the wave vectors. By taking into account the fact that the last term for $p=0$ is a constant, one can handle this equation exactly in the same way as the previous ones and again obtain (6.1).

Let us now consider the general case. Taking into account the definition of the functions $\rho'_{(\gamma)}{}^{(r)}(t)$, we have



(6.8)

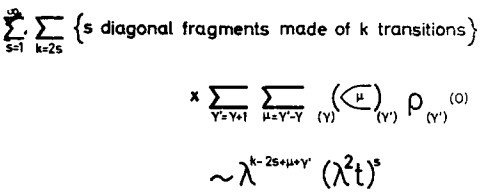
where $\eta(x)$ is the Heaviside function.

All those contributions are of the order $\lambda^{r+\gamma}$. The first one is the initial condition. The second and third one correspond to the contribution of destruction fragments. The second one is in fact an exchange fragment: the correlation (γ') contains as many particles as the correlation (γ). We have at least one of the vertices (e) or (f) of Fig. 1 in this contribution and therefore an uncompensated λ factor. This accounts for the factor $\eta(r-1)$. The factor $(1-\delta_{\gamma,0})$ accounts for the fact that such diagrams do not exist if $\gamma=0$.

In the third term, as $\gamma'>\gamma$, we must at least have one of the vertices (c) or (d) of Fig. 1. This brings at least one λ factor. As $\gamma'>\gamma$, we must at least have at our disposal a λ^2 factor which accounts for the function $\eta(r-2)$. The fourth term corresponds to the contribution of all diagonal diagrams of the required order, whereas the fifth and sixth ones correspond to the contributions of diagonal fragments preceded by a destruction fragment; they differ in the same way as the second and third do.

In order to fix the limits on the summation, one has to take account of the fact that the order of the diagram must be $\lambda^{r+\gamma}$.

Moreover, when we have a destruction fragment, we must have at least one transition in the fragment. When $\gamma'>\gamma$, we need in fact at least $(\gamma'-\gamma)$ transitions to connect the two states. Let us for instance consider more closely the last term in (6.8). The general term of this type is



(6.9)

and, therefore, we must have

$$k-2s+\mu+\gamma'=r+\gamma, \quad \mu=-k+2s+r+\gamma-\gamma'. \tag{6.10}$$

Since we must satisfy $\mu\geq\gamma'-\gamma$, we obtain the condition

$$\gamma'\leq(r-k+2s)/2+\gamma, \tag{6.11}$$

but $\gamma'\geq\gamma+1$ and, therefore,

$$k\leq r+2s-2. \tag{6.12}$$

The last three contributions in the rhs of (6.8) are the only ones which depend on time at the asymptotic limit. We can write them in another way, i.e., we can write explicitly the first diagonal fragment at the left. This can be done exactly in the same way as in footnote reference 1, and we shall not go through the details. We obtain

$$\rho'_{(\gamma)}{}^{(r)}(t) = \text{constant} + \sum_{i=0}^{r} \lambda^2 \; (i+2)_{(\gamma)} \int_0^t dt_i \, \rho_{(\gamma)}^{(r-i)}(t_i), \qquad (6.13)$$

which by derivation with respect to time gives us the very simple diagonal differential equation (6.1).

7. EVOLUTION EQUATIONS FOR THE FUNCTIONS $\rho''_{(\gamma)}{}^{(r)}(t)$ $(\gamma \geq 1)$

These functions can be expressed in terms of the functions $\rho'_{(\gamma')}{}^{(r)}(t)$ describing lower-order correlations. Let us first consider a few examples. The lowest order of these functions is $\rho''_{(1)}{}^{(0)}$ corresponding to a binary correlation.

In order to create such a correlation, we have to start from the state $\{0\}$ and use one vertex of type (a) (Fig. 1). This diagram provides the required λ factor. Therefore it can only be preceded by a succession of cycles, which add no extra λ factors uncompensated by a t factor. We thus have the equation

$$\rho''^{(0)}_{(1)}(t) = \sum_{p=0}^{\infty} (2)^p \, \rho_{0(0)} = \rho_0^{(0)}(t), \qquad (7.1)$$

where we have used (6.2).

At order λ^2, we have to consider both $\rho''_{(1)}{}^{(1)}(t)$ and $\rho''_{(2)}{}^{(0)}(t)$. The contributions to $\rho''_{(1)}{}^{(1)}(t)$ must contain one more λ factor than those in (7.1). Therefore, we must either add one vertex to the creation fragment [Fig. 1, (e) or (f)] or replace a cycle by a diagonal fragment with three vertices. We thus obtain

$$\rho''^{(1)}_{(1)}(t) = \{ \; + \; \} \left\{ \sum_{p=0}^{\infty} (2)^p \rho_{0(0)} \right\} + \; \left\{ \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} (2)^p \, 3 \, (2)^q \rho_{0(0)} \right\}$$
$$+ \; (1)\,(2)\,_{(0)} \rho_0^{(0)}(t) + (1)\,(1)\,_{(0)} \rho_0^{(1)}(t) \qquad (7.2)$$

using (6.2) and (6.3).

In the case of the function $\rho''_{(2)}{}^{(0)}(t)$, the creation fragment may start either from a binary correlation or from the state $\{0\}$. In the first case, we need a vertex of type (b), Fig. 1, whereas in the second case we need a vertex of type (b) and one of type (a).

On taking account of the initial conditions, both will lead to a λ^2 factor. Therefore they can only be preceded by cycles and we have

$$\rho''^{(0)}_{(2)}(t) = \left\{ \sum_{p=0}^{\infty} \left[(1) \right]^p \rho_{(1)(0)} \right\} + \left\{ \sum_{p=0}^{\infty} (2)^p \, \rho_{0(0)} \right\}$$
$$= (2)\,(1)\,_{(1)} \rho'^{(0)}_{(1)}(t) + (2)\,(2)\,_{(0)} \rho'^{(0)}_{(0)}(t). \qquad (7.3)$$

More complicated diagrams will occur at the next order because of the possibility of starting the diagram by a destruction fragment. This is illustrated for $\rho''_{(1)}{}^{(2)}(t)$ and $\rho''_{(2)}{}^{(1)}(t)$ in Eqs. (7.3′) and (7.3″).

$$\rho''^{(2)}_{(1)}(t) = \{ \; + \; + \; + \; + \; + \; \} (2)^p \, \rho_{0(0)}$$
$$+ \{ \; + \; \} (2)^p \, 3 \, (2)^q \rho_{0(0)} + \{ (2)^p \, 3 \, (2)^q \, 3 \, (2)^m$$
$$+ (2)^p \, 4 \, (2)^q \} \rho_{0(0)} + (2)^p \rho_{(1)(0)}, \qquad (7.3')$$

$$\rho''^{(1)}_{(2)}(t) = \{ \; + \; + \; + \cdots \} \times (2)^p \, \rho_{0(0)} + (2)^p \, 3 \, (2)^q \rho_{0(0)}$$
$$+ \{ \; + \; + \; + \; \} (2)^p \rho_{(1)(0)}$$
$$+ (2)^p \, 3 \, (2)^q \rho_{(2)(0)} + (2)^p \; + \; \} \rho_{(1)}^{(0)}. \qquad (7.3'')$$

The general equation may be written

$$\lambda^{\gamma}\rho''^{(r)}_{(\gamma)}(t)=\sum_{\gamma'=0}^{\gamma-1}\exp[-i(kv)_{\gamma'}t]\,\big(\overbrace{\quad}^{r+\gamma-\gamma'}\big)_{(\gamma)}\rho_{(\gamma')}(0)$$

$$+\sum_{\gamma'=0}^{\gamma-1}\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'-1}\exp[-i(kv)_{\gamma'}t]\,\big(\overbrace{\quad}^{\mu}\big)_{(\gamma)}\eta(r-1)(1-\delta_{\gamma',0})\,\big(\overbrace{\quad}^{r+\gamma-\mu-\gamma'}\big)_{(\gamma')}\rho_{(\gamma')}(0)$$

$$+\sum_{\gamma'=0}^{\gamma-1}\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'-2}\exp[-i(kv)_{\gamma'}t]\,\big(\overbrace{\quad}^{\mu}\big)_{(\gamma)}\eta(r-2)\sum_{\gamma''=\gamma'+1}^{(r+\gamma+\gamma'-\mu)/2}\big(\overbrace{\quad}^{r+\gamma-\mu-\gamma''}\big)_{(\gamma'')}\rho_{(\gamma'')}(0)$$

$$+\sum_{\gamma'=0}^{\gamma-1}\exp[-i(kv)_{\gamma'}t]\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'}\big(\overbrace{\quad}^{\mu}\big)_{(\gamma)}\sum_{s=1}^{\infty}\{\text{s diagonal fragments made of } (r+\gamma-\mu+2s-\gamma') \text{ transitions}\}\rho_{(\gamma')}(0)$$

$$+\sum_{\gamma'=0}^{\gamma-1}\exp[-i(kv)_{\gamma'}t]\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'-1}\big(\overbrace{\quad}^{\mu}\big)_{(\gamma)}\eta(r-1)(1-\delta_{\gamma',0})\sum_{s=1}^{\infty}\sum_{k=2s}^{r+\gamma-\mu+2s-\gamma'-1}\{\text{s diagonal fragments made of k transitions}\}\times\big(\overbrace{\quad}^{r+\gamma-\mu-k+2s-\gamma'}\big)_{(\gamma')}\rho_{(\gamma')}(0)$$

$$+\sum_{\gamma'=0}^{\gamma-1}\exp[-i(kv)_{\gamma'}t]\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'-2}\big(\overbrace{\quad}^{\mu}\big)_{(\gamma)}\sum_{s=1}^{\infty}\sum_{k=2s}^{r+\gamma-\gamma'-\mu+2s-2}\{\text{s diagonal fragments made of k transitions}\}\times\sum_{\gamma''=\gamma'+1}^{(r+\gamma+\gamma'-\mu-k+2s)/2}\big(\overbrace{\quad}^{r+\gamma-\mu-k+2s-\gamma''}\big)_{(\gamma'')}\rho_{(\gamma'')}(0). \tag{7.4}$$

The various terms correspond to the following contributions: (1) creation fragment, (2) and (3) destruction fragment followed by creation, (4) diagonal fragments followed by a creation fragment, (5) and (6) destruction fragment followed by diagonal fragments followed by a creation fragment. All these terms are of order $\lambda^{r+\gamma}$. The limits of the summations are fixed in the same manner as in Sec. 6, taking into account the supplementary conditions that there must be at least one vertex of type (a) or (b) in the creation fragment (i.e., $\gamma'<\gamma$) and the fact that the minimum number of transitions required in that fragment is $(\gamma-\gamma')$. The oscillating exponentials in front are related to free propagation of the correlation (γ'). All these terms have one common feature: the existence of the creation fragment at the left. If we take into account (6.8) and

$$\big(\overbrace{\quad}^{r+\gamma-\gamma'}\big)_{(\gamma)}=\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'}\delta_{r+\gamma-\gamma',\mu}\,\big(\overbrace{\quad}^{\mu}\big)_{(\gamma)}, \tag{7.5}$$

$$\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'-1}\eta(r-1)(1-\delta_{\gamma',0})=\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'}(1-\delta_{\gamma',0})\eta(r+\gamma-\gamma'-\mu-1), \tag{7.6}$$

$$\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'-2}\eta(r-2)=\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'}\eta(r+\gamma-\gamma'-\mu-2), \tag{7.7}$$

equation (5.1) can be rewritten

$$\rho''^{(r)}_{(\gamma)}(t)=\sum_{\gamma'=0}^{\gamma-1}\sum_{\mu=\gamma-\gamma'}^{r+\gamma-\gamma'}\exp[-i(kv)_{\gamma'}t]\,\big(\overbrace{\quad}^{\mu}\big)_{(\gamma)}\rho'^{(r+\gamma-\gamma'-\mu)}_{(\gamma')}(t)$$

$$=\sum_{\gamma'=0}^{\gamma-1}\sum_{\nu=0}^{r}\exp[-i(kv)_{\gamma'}t]\,\big(\overbrace{\quad}^{\nu+\gamma-\gamma'}\big)_{(\gamma)}\rho'^{(r-\nu)}_{(\gamma')}(t). \tag{7.8}$$

This equation gives us the functions $\rho''^{(r)}_{(\gamma)}(t)$ in terms of the functions $\rho'^{(r-\nu)}_{(\gamma')}(t)$ which describe lower correlations.

8. EQUILIBRIUM DISTRIBUTION

For systems of interacting particles, the interaction forces are often strong and the relevant expansion parameter is the concentration C.

Let us consider the canonical equilibrium distribution

$$\rho^{\text{equ}}=\frac{\exp[-\beta(H_0+\lambda V)]}{\int\int(drdp)^N\exp[-\beta(H_0+\lambda V)]}. \tag{8.1}$$

Expansions of (8.1) in power series of the concentration have been extensively studied in equilibrium statistical mechanics.[5,6] As the potential is independent of the velocities, the equilibrium velocity distribution function is always given by

$$\rho_0^{\text{equ}}=\int(dr)^N\rho^{\text{equ}}=(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0), \tag{8.2}$$

whatever the order in C or λ.

The pair correlation function is given by[7]:

$$g(r_{12})=\Omega^2\int(dp)^N\int dr_3\cdots dr_N\,\rho^{\text{equ}}$$

$$=\exp[-\beta V(r_{12})]\times[1+\sum_{k=1}^{\infty}C^k\gamma_k(r_{12})] \tag{8.3}$$

[5] J. Van Leeuwen, J. Groenenveld, and J. de Boer, Physica **25**, 792 (1959).

[6] E. Meeron, Phys. Fluids **1**, 130 (1958).

[7] We use here the definitions given by J. Van Leeuwen, J. Groenenveld, and J. de Boer in footnote reference 5.

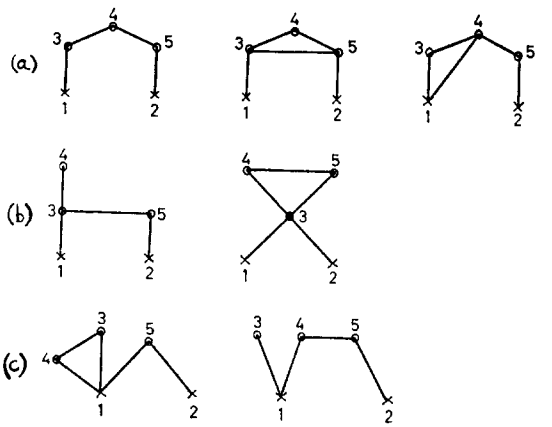


FIG. 8. Examples of cluster diagrams corresponding to products of f_{ij}'s in (8.5). (a) Irreducible diagrams, (b) 3≡articulation point, (c) 1≡articulation point.

with

$$\gamma_k(r_{12})=\frac{1}{k!}\int\cdots\int\sum_{\text{(sp. irr.)}}\prod f(r_{ij})dr_3\cdots dr_{k+2}, \quad (8.4)$$

$$f(r_{ij})=\exp[-\beta V(r_{ij})]-1. \quad (8.5)$$

The summation in (8.4) is carried out over all different products of factors $f(r_{ij})$ excluding $f(r_{12})$ itself, provided the product corresponds to a "specific irreducible 1–2 diagram." Such diagrams are cluster diagrams with two reference points 1 and 2 and k numbered (distinguishable) points $3,4\cdots k+2$ which are connected by a certain number of bonds, each bond corresponding to one of the factor $f(r_{ij})$ in the product considered. Such a diagram is called irreducible when it is a connected diagram [not containing the direct bond (1–2)] which has no articulation point. Examples are given in Fig. 8.

At equilibrium the Fourier coefficient $\rho_{(1)}$ describing a correlation between particles 1 and 2 is given by [see (2.4)]

$$\Omega^{-1}[\rho_l{}^1{}_{-l}{}^2\exp(ilv_{12}t)]_{\text{equ}}$$
$$=\int(dr)^N\exp(-ilr_{12})\rho^{\text{equ}}$$
$$=\Omega^{-1}(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0)\int dr_{12}$$
$$\times\exp(-ilr_{12})g(r_{12}). \quad (8.6)$$

This Fourier coefficient leads to contributions to intensive variables which are at least of order C. Indeed, if we consider for instance the contribution to the mean value of the potential energy per particle, we obtain

$$\frac{\langle E\rangle}{N}=N^{-1}\sum_{ij}\int(dr)^N V_{ij}(r_{ij})\rho^{\text{equ}}$$
$$=(N\Omega)^{-1}\sum\int dr_{ij}\int dl\exp(ilr_{ij})V_{ij}$$
$$\times[\rho_l{}^i{}_{-l}{}^j\exp(ilv_{ij}t)]_{\text{equ}}=O(N^2/N\Omega)=O(C).$$

In the same meaning, the Fourier coefficients $\rho_{(\gamma)}$ which describe correlations between $(\gamma+1)$ particles have to be taken into account at order C^r, $r\geqslant\gamma$.

Let us consider more closely the contributions to the equilibrium distribution up to order C^2. At order C^0, the system is entirely described by the velocity distribution function

$$\rho_0{}^{\text{equ}}=(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0). \quad (8.7)$$

At order C, we have to take into account the lowest-order contribution to $\rho_{(1)}$:

$$[\rho_{(1)}\exp(ilv_{12}t)]_C$$
$$=(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0)\int dr_{12}\exp(-ilr_{12})$$
$$\times\exp(-\beta\lambda V_{12}). \quad (8.8)$$

The factor $\exp(-\beta\lambda V_{12})$ can be expanded in power series of the coupling constant λ. Therefore the contributions of order $C\lambda^s$ will be

$$[\rho_{(1)}{}^{(s)}\exp(ilv_{12}t)]_C$$
$$=(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0)\int dr_{12}\exp(-ilr_{12})$$
$$\times(-\beta V_{12})^s/s!. \quad (8.9)$$

At order C^2, we have to take into account the next contribution to $\rho_{(1)}$:

$$[\rho_{(1)}\exp(ilv_{12}t)]_{C^2}$$
$$=C(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0)\int dr_{12}\exp(-ilr_{12})$$
$$\times\gamma_1(r_{12})\exp(-\beta\lambda V_{12}), \quad (8.10)$$

with

$$\gamma_1(r_{12})=\int dr_3 f(r_{13})f(r_{23}), \quad (8.11)$$

and the first-order contribution to the three-particle correlation

$$[\rho_{(2)}\exp\{-i(l_1v_1+l_2v_2+l_3v_3)t\}]_{C^2}$$
$$=(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0)\int dr_{12}dr_{13}$$
$$\times\exp[-i(l_1r_1+l_2r_2+l_3r_3)]$$
$$\times\exp[-\beta\lambda(V_{12}+V_{13}+V_{23})]$$

with

$$l_1+l_2+l_3=0. \quad (8.12)$$

Both (8.10) and (8.12) can be expanded in power series of λ. The contributions at order λ^sC^2 are then given by

$$[\rho_{(1)}{}^{(s)}\exp(-ilv_{12}t)]_{C^2}$$
$$=C(\pi\beta^{-1})^{3N/2}\exp(-\beta H_0)\int dr_{12}\exp(-ilr_{12})$$
$$\times\int dr_3\sum_{p=0}^{s-2}\sum_{q=0}^{s-p-1}\frac{(-\beta)^s}{p!q!(s-p-q)!}$$
$$\times V_{12}{}^pV_{13}{}^qV_{23}{}^{s-p-q} \quad (8.13)$$

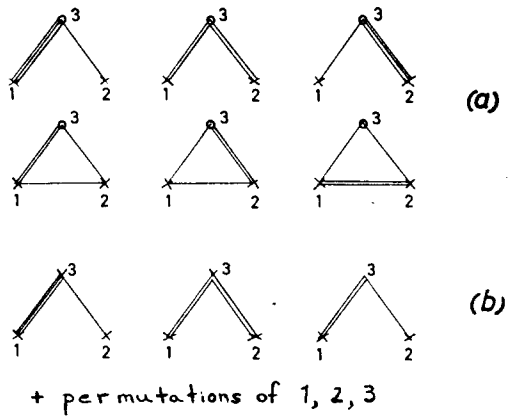


FIG. 9. Equilibrium diagrams at order $C^2\lambda^4$. (a) Contributions to the binary correlation 1–2, (b) contributions to the triple correlation 1–2–3.

and

$$[\rho_{(2)}{}^{(s)} \exp\{-i(l_1v_1+l_2v_2+l_3v_3)t\}]_{C^2}$$
$$= (\pi\beta^{-1})^{3N/2} \exp(-\beta H_0) \int dr_{12}dr_{13} \times \exp[-i(l_1r_1+l_2r_2+l_3r_3)] \frac{(-\beta)^s}{s!} \times (V_{12}+V_{13}+V_{23})^s. \quad (8.14)$$

These contributions can be represented graphically in a way very similar to the diagrams in Fig. 8; however, each bond between two particles will now correspond to a factor V_{ij}, instead of a factor f_{ij} as in Fig. 8. Examples are given in Fig. 9.

9. APPROACH TO EQUILIBRIUM—VELOCITY DISTRIBUTION FUNCTION

This function is given by (6.7) for $\gamma=0$:

$$\partial\rho_0^{(r)}/\partial t = \lambda^2 \sum_{i=0}^{r} \textcircled{i+2} \rho_0^{(r-i)}(t). \quad (9.1)$$

At lowest order in λ ($r=0$), we have the master equation for weakly coupled systems[2]:

$$\partial\rho_0^{(0)}/\partial t = \lambda^2 \textcircled{2} \rho_0^{(0)}(t). \quad (9.2)$$

The operator associated with the cycle is a self-adjoint operator with negative eigenvalues. The eigenfunction corresponding to the eigenvalue zero is a function of the unperturbed Hamiltonian H_0. Therefore, for long times,

$$\rho_0{}^{(0)} \to f(H_0). \quad (9.3)$$

We can use this result to study the next approximation:

$$\partial\rho_0^{(1)}/\partial t = \lambda^2 \textcircled{2} \rho_0^{(1)} + \lambda^2 \textcircled{3} \rho_0^{(0)}, \quad (9.4)$$
$$= \lambda^2 \textcircled{2} \rho_0^{(1)} + \lambda^2 \textcircled{3} f(H_0). \quad (9.5)$$

We shall show that the second term in the rhs vanishes. Therefore, we can study (9.5) in the same way as (9.2) and obtain

$$\rho_0{}^{(1)} \to g(H_0). \quad (9.6)$$

We can go on with this procedure. We shall obtain the required result

$$\rho_0 \to F(H_0), \quad (9.7)$$

provided we can establish the following relation:

$$\textcircled{m} \varphi(H_0) = 0 \quad (9.8)$$

for any value of $m>2$ (φ arbitrary function).

The diagonal fragments with m vertices can be further classified according to the number of particles ν which appear in the fragment ($2 \leqslant \nu \leqslant m$). Let us denote by an indice ν a diagonal fragment with m vertices in which at most ν particles appear. Rather than (9.8), we shall establish the more precise relation

$$(\textcircled{m})_\nu \varphi(H_0) = 0 \quad (9.9)$$

Equation (9.8) will be obtained from (9.9) for $\nu=m$. This relation is in fact more interesting than (9.8). Indeed, if the interaction forces are strong, the relevant parameter is the concentration. To obtain a description of the system in that case, we should have to write

$$\rho_0(t) = \sum_{r=0}^{\infty} \lambda^r \rho_0{}^{(r)}(t), \quad (9.10)$$

and expand this function with respect to C, with the condition Ct finite (instead of $\lambda^2 t$). This can be done by taking into account the fact that the order in C of a diagram is related to the number of particles which appear in this diagram. For instance, at order C^0, the evolution of $\rho_0(t)$ would be given by all the diagrams for which $\nu=2$, whatever the number of vertices[8] (sum over m from 2 to ∞). Therefore whatever the relevant parameter, λ or C, (9.9) will ensure the proper asymptotic behavior of the velocity distribution function. If we take into account the fact that to each vertex of a diagram in which at most ν particles appear corresponds a matrix element of the form

$$\langle l_1 l_2 \cdots l_\nu | \delta L^{(\nu)} | l_1' l_2' \cdots l_\nu' \rangle$$
$$= \int (dx)^\nu \exp[-i \sum_{j=1}^{\nu} l_j x_j] \sum_{j<m=1}^{\nu} (\partial V_{jm}/\partial x_j) D_{jm} \times \exp[i \sum_{j=1}^{\nu} l_j' x_j] \quad (9.11)$$

with

$$D_{jm} = (\partial/\partial v_j - \partial/\partial v_m), \quad (9.12)$$

and that to each time interval between two vertices

[8] I. Prigogine and F. Henin, Physica **24**, 214 (1958).

corresponds a propagator of the form (see Appendix)[9]

$$[i(\sum_{j=1}^{\nu} l_j v_j - i\epsilon)]^{-1}$$

$$\times \int (dx)^\nu G^{(\nu)}(x_1 \cdots x_\nu v_1 \cdots v_\nu) \exp[-i \sum_{j=1}^{\nu} l_j x_j] \quad (9.13)$$

with

$$G^{(\nu)}(\{x\}\{v\}) = \int (dl)^\nu [i(\sum_{j=1}^{\nu} l_j v_j - i\epsilon)]^{-1} \exp[i \sum_{j=1}^{\nu} l_j x_j]$$

$$= \int_0^\infty d\tau \prod_{j=1}^{\nu} \delta(x_j - v_j \tau), \quad (9.14)$$

the lhs of (9.9) can be written ($2 \leqslant \nu \leqslant m$)

$$\sum_{\{l^{(1)}\} \cdots \{l^{(m-1)}\}} \langle\{0\}|\delta L^{(\nu)}|\{l^{(1)}\}\rangle\langle\{l^{(1)}\}|G^{(\nu)}|\{l^{(1)}\}\rangle$$
$$\times \langle\{l^{(1)}\}|\delta L^{(\nu)}|\{l^{(2)}\}\rangle\langle\{l^{(2)}\}|G^{(\nu)}|\{l^{(2)}\}\rangle \cdots$$
$$\times \langle\{l^{(m-1)}\}|G^{(\nu)}|\{l^{(m-1)}\}\rangle\langle\{l^{(m-1)}\}|\delta L^{(\nu)}|\{0\}\rangle f(H_0)$$

$$= \sum_{\{l^{(1)}\} \cdots \{l^{(m-1)}\}} \int (dx^{(1)})^\nu (dx^{(2)})^\nu \cdots (dx^{(2m-1)})^\nu$$
$$\times \{\sum_{j<m=1}^{\nu} [\partial V_{jm}(x_{jm}{}^{(1)})/\partial x_j{}^{(1)}] D_{jm}\}$$
$$\times \exp[i \textstyle\sum_j l_j{}^{(1)} x_j{}^{(1)}] \exp[-i \sum_j l_j{}^{(1)} x_j{}^{(2)}]$$
$$\times G^{(\nu)}(\{x_j{}^{(2)}\}\{v_j\}) \exp[-i \textstyle\sum_j l_j{}^{(1)} x_j{}^{(3)}]$$
$$\times \{\sum_{j<m} [\partial V_{jm}(x_{jm}{}^{(3)})/\partial x_j{}^{(3)}] D_{jm}\}$$
$$\times \exp[i \textstyle\sum_j l_j{}^{(2)} x_j{}^{(3)}] \cdots G^{(\nu)}(\{x_j{}^{(2m-2)}\}\{v_j\}$$
$$\times \exp[-i \textstyle\sum_j l_j{}^{(m-1)} x_j{}^{(2m-2)}]$$
$$\times \exp[i \textstyle\sum_j l_j{}^{(m-1)} x_j{}^{(2m-1)}]$$
$$\times \{\sum_{j<m} [\partial V_{jm}(x_{jm}{}^{(2m-1)})/\partial x_j{}^{(2m-1)}] D_{jm}\} f(H_0), \quad (9.15)$$

where each set of $\{l^{(j)}\}$'s corresponds to $l_1{}^{(j)} l_2{}^{(j)} \cdots l_\nu{}^{(j)}$. The summations over the l's can be transformed into integrals which can be performed immediately.

$$\sum_{\{l^{(1)}\} \cdots \{l^{(m-1)}\}} \exp[i \textstyle\sum l_j{}^{(1)} (x_j{}^{(1)} - x_j{}^{(2)} - x_j{}^{(3)})]$$
$$\times \exp[i \textstyle\sum l_j{}^{(2)} (x_j{}^{(3)} - x_j{}^{(4)} - x_j{}^{(5)})] \cdots$$
$$\times \exp[i \textstyle\sum l_j{}^{(m-1)} (x_j{}^{(2m-3)} - x_j{}^{(2m-2)} - x_j{}^{(2m-1)})]$$

$$= \Omega^{-\nu} \prod_{j=1}^{\nu} \delta(x_j{}^{(1)} - x_j{}^{(2)} - x_j{}^{(3)}) \delta(x_j{}^{(3)} - x_j{}^{(4)} - x_j{}^{(5)}) \cdots$$
$$\times \delta(x_j{}^{(2m-3)} - x_j{}^{(2m-2)} - x_j{}^{(2m-1)}). \quad (9.16)$$

[9] P. Résibois, Physica **25**, 725 (1959).

This result can now be used in (9.15) to perform the integrations over all $x_j{}^{(2l)}$. We then obtain

$$\Omega^{-\nu} \int (dx^{(1)})^\nu \cdots (dx^{(m)})^\nu$$
$$\times \{\sum_{j<m=1}^{\nu} [\partial V_{jm}(x_{jm}{}^{(1)})/\partial x_j{}^{(1)}] D_{jm}\}$$
$$\times G^{(\nu)}(\{x_j{}^{(1)} - x_j{}^{(2)}\}\{v_j\})$$
$$\times \{\sum_{j<m} [\partial V_{jm}(x_{jm}{}^{(2)})/\partial x_j{}^{(2)}] D_{jm}\} \cdots$$
$$\times G^{(\nu)}(\{x_j{}^{(m-2)} - x_j{}^{(m-1)}\}\{v_j\})$$
$$\times \{\sum_{j<m} [\partial V_{jm}(x_{jm}{}^{(m-1)})/\partial x_j{}^{(m-1)}] D_{jm}\}$$
$$\times G^{(\nu)}(\{x_j{}^{(m-1)} - x_j{}^{(m)}\}\{v_j\})$$
$$\times \{\sum_{j<m} [\partial V_{jm}(x_{jm}{}^{(m)})/\partial x_j{}^{(m)}] D_{jm}\} f(H_0). \quad (9.17)$$

In order to study this expression, we shall make use of the following relations:

$$\frac{1}{s!} [\sum_{j<m} V_{jm}]^s \{\sum_{j<m} [\partial V_{jm}(x_{jm})/\partial x_j] D_{jm}\} f(H_0)$$
$$= [\partial f/\partial H_0] \frac{1}{s!} [\sum_{j<m} V_{jm}]^s \{\sum_{j<m} [\partial V_{jm}/\partial x_j] v_{jm}\}$$
$$= [\partial f/\partial H_0] \frac{1}{s!} [\sum_{j<m} V_{jm}]^s \sum_{t=1}^{\nu} v_t \frac{\partial}{\partial x_t} [\sum_{j<m} V_{jm}]$$
$$= [\partial f/\partial H_0] \frac{1}{(s+1)!} \sum_{t=1}^{\nu} v_t \frac{\partial}{\partial x_t} [\sum_{j<m} V_{jm}]^{s+1} \quad (9.18)$$

and

$$\sum_{t=1}^{\nu} v_t \frac{\partial}{\partial x_t} G^{(\nu)}(\{x_j - x_j'\}\{v_j\}) = \prod_{j=1}^{\nu} \delta(x_j - x_j') \quad (9.19)$$

as can be seen from (9.14).

Let us for instance consider the two last factors in (9.17). We have

$$\int (dx^{(m)})^\nu G^{(\nu)}(\{x_j{}^{(m-1)} - x_j{}^{(m)}\}\{v_j\}) \times \sum_{j<m} [\partial V_{jm}(x_{jm}{}^{(m)})/\partial x_j{}^{(m)}] D_{jm} f(H_0)$$
$$= [\partial f/\partial H_0] \int (dx^{(m)})^\nu G^{(\nu)}(\{x_j{}^{(m-1)} - x_j{}^{(m)}\}\{v_j\}) \times \sum_{t=1}^{\nu} v_t \frac{\partial}{\partial x_t{}^{(m)}} [\sum_{j<m} V_{jm}(x_{jm}{}^{(m)})]$$
$$= -[\partial f/\partial H_0] \int (dx^{(m)})^\nu [\sum_{j<m} V_{jm}(x_{jm}{}^{(m)})] \times \sum_{t=1}^{\nu} v_t \frac{\partial}{\partial x_t{}^{(m)}} G^{(\nu)}(\{x_j{}^{(m-1)} - x_j{}^{(m)}\}\{v_j\})$$
$$= -[\partial f/\partial H_0][\sum_{j<m} V_{jm}(x_{jm}{}^{(m-1)})], \quad (9.20)$$

where we have first used (9.18), then integrated by parts and finally used (9.19) and performed the integral over the $x^{(m)}$. One can go on step by step following the same procedure. One then obtains

$$\Omega^{-\nu}\int (dx^{(1)})^{\nu}[\partial^m f/\partial H_0{}^m]\frac{1}{m!}\sum_{i=1}^{\nu} v_i\frac{\partial}{\partial x_i{}^{(1)}}$$

$$\times[\sum_{j<m}^{\nu} V_{jm}(x_{jm}{}^{(1)})]=0, \quad (9.22)$$

which establishes (9.9) and therefore the H theorem for the velocity distribution function.

10. ASYMPTOTIC BEHAVIOR OF THE FUNCTIONS $\varrho'_{(\gamma)}{}^{(r)}(t)$

Here again we shall first consider the lowest-order contribution to these functions ($r=0$). Then we have the equation

$$\partial\rho'^{(0)}_{(\gamma)}/\partial t=\lambda^2\,(\gamma)\,\textcircled{2}\,(\gamma)\,\rho'^{(0)}_{(\gamma)}(t). \quad (10.1)$$

It has been shown[4] that for long times this equation leads to

$$\rho'_{(\gamma)}{}^{(0)}\to 0. \quad (10.2)$$

On using this result at the next order, we obtain

$$\partial\rho'^{(1)}_{(\gamma)}/\partial t=\lambda^2\,(\gamma)\,\textcircled{2}\,(\gamma)\,\rho'^{(1)}_{(\gamma)}(t), \quad (10.3)$$

and therefore

$$\rho'_{(\gamma)}{}^{(1)}\to 0. \quad (10.4)$$

This procedure can be followed up to any order. The asymptotic solution of the set of Eqs. (6.7) for $\gamma\neq 0$ is then

$$\rho'_{(\gamma)}\to 0. \quad (10.5)$$

In other words, the contribution of scattering of particles to the evolution of the phase correlation $\rho_{(\gamma)}(t)$ vanishes after a long time.

11. ASYMPTOTIC BEHAVIOR OF THE FUNCTIONS $\varrho''_{(\gamma)}{}^{(r)}(t)$ ($\gamma\geq 1$)—APPROACH TO EQUILIBRIUM AT ORDER C

After a long time, we can use (9.7) and (10.5) in (7.5). If we take for ρ_0 the canonical distribution, we have

$$\rho''^{(r)}_{(\gamma)}(t)\to(\gamma)\,\textcircled{\gamma\gamma}\,(0)\,(\pi\beta^{-1})^{3N/2}\exp[-\beta H_0]. \quad (11.1)$$

This means that after a long time, the only contributions to the phase correlation $\rho_{(\gamma)}(t)$ come from the terms where this correlation is built from the state $\{0\}$. At this point, we can see that the decomposition of the phase correlation $\rho_{(\gamma)}(t)$ into two parts, $\rho'_{(\gamma)}$ and $\rho''_{(\gamma)}$, is actually a very important feature of the theory; without the great simplifications introduced by this procedure, it would be very hard to establish any general properties at all.

In order to have a complete H theorem, we have to show that (11.1) is identical with the equilibrium distribution. Equation (11.1) corresponds to the case where λ is the relevant parameter; however, we can follow the procedure explained in Sec. 9 to obtain the equations if we want to use C as a parameter. At order $C^m\lambda^s$ we shall then have the equations

$$[\rho^{(s)}_{(\gamma)}]_{Cm}\to\{(\gamma)\,\textcircled{s}\,(0)\}_{(m+1)}(\pi\beta^{-1})^{3N/2}\exp[-\beta H_0] \quad (11.2)$$

for all values of γ and s such that

$$1\leqslant\gamma\leqslant m\leqslant s.$$

The subscript $(m+1)$ means that we have only to keep the diagrams where $(m+1)$ particles appear. In order to establish that (11.2) corresponds to the correct equilibrium diagrams at order $C^m\lambda^s$ we shall follow the same procedure as in Sec. 9; however, the proof will not be so straightforward. Indeed, in the case of the velocity distribution function, all the particles which appear in the diagram play the same role, whereas in (11.2) we have two groups of particles: first the $(\gamma+1)$ particles which are correlated and then the $(m-\gamma)$ particles which appear at one vertex of the diagram and disappear at another one and which we shall call dummy particles.

Let us first consider how the equilibrium distribution will be obtained at order C. We have to study only correlations between 2 particles, which we shall denote by 1 and 2. No dummy particles appear at this order. The only diagrams we have are given in Fig. 10. They correspond to successive Born approximations. We have

$$[\rho_{(1)}{}^{(s)}]_C\to(\pi\beta^{-1})^{3N/2}\langle l|G^{(1,2)}|l\rangle$$

$$\times\sum_{l^{(1)}\cdots l^{(s-1)}}\langle l|\delta L_{12}|l^{(1)}\rangle\langle l^{(1)}|G^{(1,2)}|l^{(1)}\rangle$$

$$\times\langle l^{(1)}|\delta L_{12}|l^{(2)}\rangle\cdots\langle l^{(s-1)}|\delta L_{12}|0\rangle\exp[-\beta H_0]. \quad (11.3)$$

On taking account of (9.11) and (9.14) and following

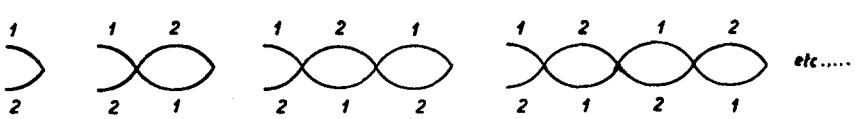


FIG. 10. Creation fragments contributing to the equilibrium pair correlation at order C.

the same procedure as used to obtain (9.17), we obtain

$$[\rho_{(1)}{}^{(s)}]_C \to (\pi\beta^{-1})^{3N/2}\Omega^{-1}\langle l|G^{(1,2)}|l\rangle \times\int dx^{(1)}\cdots dx^{(s)}\exp[-ilx_{12}{}^{(1)}](\partial V_{12}/\partial x_1{}^{(1)})D_{12} \times G^{(1,2)}(x^{(1)}-x^{(2)})(\partial V_{12}/\partial x_1{}^{(2)})D_{12}\cdots \times G^{(1,2)}(x^{(s-1)}-x^{(s)})(\partial V_{12}/\partial x_1{}^{(s)})D_{12}\exp[-\beta H_0]$$

$$=(\pi\beta^{-1})^{3N/2}\Omega^{-1}\frac{(-\beta)^s}{s!}\exp[-\beta H_0]\langle l|G^{(1,2)}|l\rangle \times\int dx_1dx_2\exp[-ilx_{12}](\partial[V_{12}]^s/\partial x_1)\cdot v_{12}. \quad (11.4)$$

On integrating by parts and taking into account

$$il\cdot v_{12}\langle l|G^{(1,2)}|l\rangle=\frac{il\cdot v_{12}}{i(l\cdot v_{12}-i\epsilon)}=1, \quad (11.5)$$

we obtain

$$[\rho_{(1)}{}^{(s)}]_C \to (\pi\beta^{-1})^{3N/2}\frac{(-\beta)^s}{s!}\Omega^{-1}\exp[-\beta H_0] \times\int dx_1dx_2V_{12}{}^s\exp(-ilx_{12})$$

$$=(\pi\beta^{-1})^{3N/2}\frac{(-\beta)^s}{s!}\exp[-\beta H_0] \times\int dx_{12}V_{12}{}^s\exp(-ilx_{12}) \quad (11.6)$$

in complete agreement with (8.9).

12. APPROACH TO EQUILIBRIUM AT ORDER C^2

We shall first study the correlation between two particles 1 and 2. All our diagrams must contain, besides the particles 1 and 2, one dummy particle 3. To each diagram with s vertices will correspond an expression of the form

$$(\pi\beta^{-1})^{3N/2}\Omega^{-2}\langle l|G^{(1,2)}|l\rangle\int dx^{(1)}\cdots dx^{(s)} \times(\partial V_{ij}/\partial x_i{}^{(1)})D_{ij}G^{(123)}(x^{(1)}-x^{(2)})(\partial V_{kl}/\partial x_k{}^{(2)}) \times D_{kl}G^{(123)}(x^{(2)}-x^{(3)})\cdots(\partial V_{mn}/\partial x_m{}^{(s)})D_{mn} \times\exp[-\beta H_0], \quad (12.1)$$

where the V_{ij}'s, etc....are either V_{12}, V_{13}, or V_{23} according to the particular diagram we consider.

As a matter of fact, when we consider a particular diagram, some of the integrals in (12.1) can be trivially performed. Indeed, in Fourier space, the wave vector $\mathbf{k}=\mathbf{0}$ plays a special role. Equation (12.1) is a general expression which does not take account of this fact explicitly; however, this can be done easily, taking into account the fact that if the n first vertices at the right involve only 2 particles, we can integrate immediately over the coordinates $x_i{}^{(s-n)}x_i{}^{(s-n-1)}\cdots x_i{}^{(s)}$ of the third particle, taking into account

$$\int dx_i'dx_j'dx_k'G^{(ijk)}(x_i-x_i',x_j-x_j',x_k-x_k') \times f(x_ix_jx_kx_j'x_k') =\int dx_j'dx_k'G^{(jk)}(x_j-x_j',x_k-x_k') \times f(x_ix_jx_kx_j'x_k'). \quad (12.2)$$

Similarly, if the dummy particle 3 disappears at the mth vertex, we can integrate immediately over $x_3{}^{(1)}\cdots x_3{}^{(m-1)}$. In each case, the 3-particles propagator reduces to 2-particles propagator to or from the vertex concerned. This corresponds to the fact that to or from that vertex we have only a 2-body interaction.

Let us now consider more closely the structure of the diagrams. At the first vertex on the right, we can have any of the 3 interactions 12, 13, or 23. In each case we have

$$-\beta\int dx_1{}^{(s)}dx_2{}^{(s)}dx_3{}^{(s)}G^{(123)}(x^{(s-1)}-x^{(s)}) \times(\partial V_{mn}/\partial x_m{}^{(s)})v_{mn}\exp[-\beta H_0] =-\beta\exp[-\beta H_0]V_{mn}(x_{mn}{}^{(s-1)}). \quad (12.3)$$

At any vertex k ($2\leqslant k\leqslant s-2$), we can subdivide the diagrams into three classes:

A. 3 has not yet appeared in the diagram.

B. 3 appears at the left of the diagram, being created at the kth vertex or earlier in the diagram.

C. 3 has appeared in the diagram but has been destroyed either at the kth vertex or earlier in the diagram.

All possible diagrams at the second vertex are given in Fig. 11. In Fig. 12 we give some examples of the 3 classes of diagrams for $k=4$.

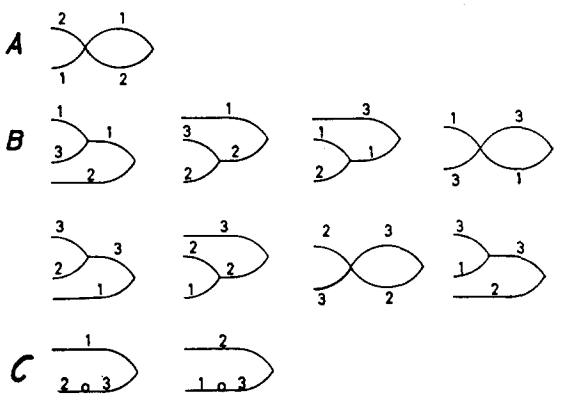


FIG. 11. All possible diagrams at the second vertex.

For the diagrams of class A at the second vertex, we obtain after integration over $dx^{(s-1)}$

$$\cdots\frac{V_{12}^2(x_{12}^{(s-1)})}{2!}(-\beta)^2\exp[-\beta H_0]. \quad (12.4)$$

For the eight diagrams of class B at the second vertex, we have

$$\begin{aligned}\cdots(-\beta)^2\int dx^{(s-1)}G^{(123)}(x^{(s-2)}-x^{(s-1)})&\\ \times\{V_{12}(x_{12}^{(s-1)})[(\partial V_{13}/\partial x_1^{(s-1)})v_{13}&\\ +(\partial V_{23}/\partial x_2^{(s-1)})v_{23}]+[V_{13}(x_{13}^{(s-1)})&\\ +V_{23}(x_{23}^{(s-1)})][(\partial V_{12}/\partial x_1^{(s-1)})v_{12}&\\ +(\partial V_{13}/\partial x_1^{(s-1)})v_{13}+(\partial V_{23}/\partial x_2^{(s-1)})v_{23}]\}&\\ \times\exp[-\beta H_0]&\\ =\cdots(-\beta)^2\exp[-\beta H_0]\int dx^{(s-1)}G^{(123)}(x^{(s-2)}-x^{(s-1)})&\\ \times\{\sum_{t=1}^{3}v_t\partial/\partial x_t^{(s-1)}\}\{V_{12}(V_{13}+V_{23})&\\ +(1/2!)(V_{13}+V_{23})^2\}_{x^{(s-1)}}&\\ =\cdots(-\beta)^2\exp[-\beta H_0]\{V_{12}(V_{13}+V_{23})&\\ +(1/2!)(V_{13}+V_{23})^2\}_{x^{(s-2)}}&\\ =\cdots(-\beta)^2\exp[-\beta H_0]\{(1/2!)(V_{12}+V_{13}+V_{23})^2&\\ -(1/2!)V_{12}^2\}_{x^{(s-2)}}. \quad (12.5)\end{aligned}$$

For the two diagrams of class C at the second vertex, we have

$$\begin{aligned}\cdots(-\beta)^2\exp[-\beta H_0]\int dx^{(s-1)}G^{(123)}(x^{(s-2)}-x^{(s-1)})&\\ \times\{V_{23}(x_{23}^{(s-1)})[\partial V_{13}/\partial x_1^{(s-1)}]v_{13}+V_{13}&\\ \times[\partial V_{23}/\partial x_2^{(s-1)}]v_{23}\}&\\ =\cdots(-\beta)^2\exp[-\beta H_0]\{V_{13}V_{23}\}_{x^{(s-2)}}. \quad (12.6)\end{aligned}$$

We may notice that if $s=2$, these last two diagrams would be the only diagrams. In that case the lhs of (10.12) would have been

$$\begin{aligned}(\pi\beta^{-1})^{3N/2}\Omega^{-2}\langle l|G^{(1,2)}|l\rangle(-\beta)^2\exp[-\beta H_0]&\\ \times\int dx_1dx_2dx_3\exp(-ilx_{12})\{V_{23}(\partial V_{13}/\partial x_1)v_{13}&\\ +V_{13}(\partial V_{23}/\partial x_2)v_{23}\}&\\ =(\pi\beta^{-1})^{3N/2}\Omega^{-1}(-\beta)^2\exp[-\beta H_0]&\\ \times\int dx_{12}\exp(-ilx_{12})\int dx_3V_{13}V_{23} \quad (12.7)\end{aligned}$$

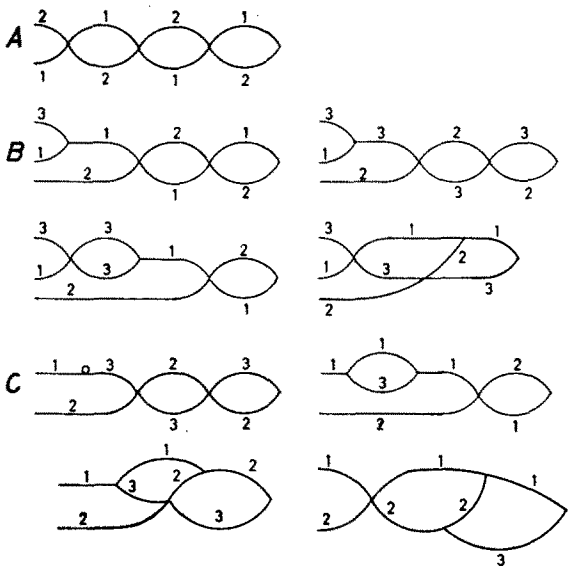


FIG. 12. Examples of diagrams at the fourth vertex.

which agrees with (8.13) for $s=2$ if we take into account the fact that 3 may be any of the $(N-2)$ particles of the system and we have to sum over all these possibilities.

The results (12.4)–(12.6) can be generalized for the three classes of diagrams at any vertex k $(k\leqslant s-2)$. One has for the diagrams at that vertex

$$\text{A.}\quad(-\beta)^k\exp[-\beta H_0](1/k!)V_{12}^k, \quad (12.8)$$

$$\begin{aligned}\text{B.}\quad(-\beta)^k\exp[-\beta H_0](1/k!)&\\ \times\{(V_{12}+V_{13}+V_{23})^k-V_{12}^k\}&\\ =(-\beta)^k\exp[-\beta H_0]\sum_{p=0}^{k-1}\frac{1}{p!(k-p)!}V_{12}^p&\\ \times(V_{13}+V_{23})^{k-p}, \quad (12.9)\end{aligned}$$

$$\begin{aligned}\text{C.}\quad(-\beta)^k\exp[-\beta H_0]\sum_{p=0}^{k-2}\frac{1}{p!(k-p)!}V_{12}^p&\\ \times\{(V_{13}+V_{23})^{k-p}-(V_{13}^{k-p}+V_{23}^{k-p})\}, \quad (12.10)\end{aligned}$$

where all V_{ij} have to be taken at the point x corresponding to the $(k+1)$th vertex.

These results are easily understood. Equation (12.8) corresponds to the fact that up to the kth vertex, we have only had a 2-body (1.2) interaction. This result is straightforward and has been established at order C. Equation (12.9) corresponds to the fact that in the diagrams of this class we may at any vertex use any of the interactions 12, 13 or 23 provided we use 13 or 23 at least once $(k-p\geqslant 1$ in the rhs).

The first term in (12.10) corresponds to the fact that in the diagrams of this class, we may also use at any vertex any of the interactions 12, 13, or 23 provided 3 has been used at least twice $(k-p\geqslant 2)$. The terms

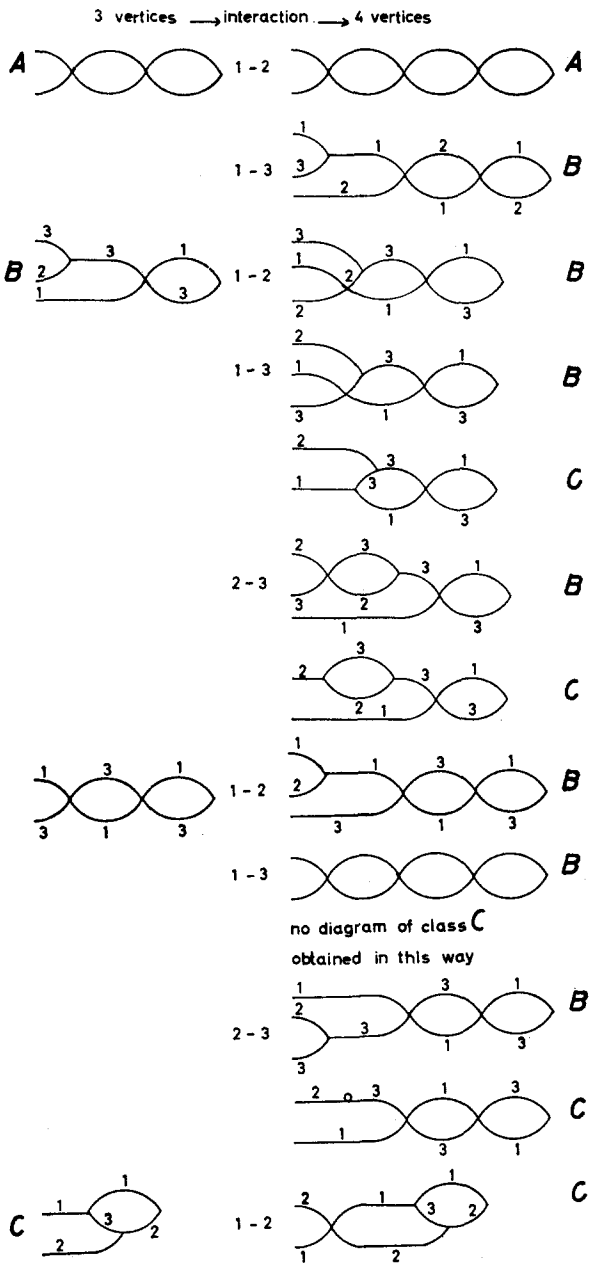


FIG. 13. Illustration of Table I.

which are subtracted correspond to diagrams which give a vanishing contribution. This can be easily understood. Indeed, in any of the corresponding diagrams, 3 has interacted with only *one* of the 2 fixed particles. As 3 will no longer play a role in the diagram, such terms should lead to cluster diagrams with that fixed particle being an articulation point.

In order to prove (12.9) and (12.10) we shall assume these results to be true at the kth vertex and prove them for the $(k+1)$th vertex. (We have already shown they are true for $k=2$.) To do this, we first have to see what

TABLE I.

Class of diagram at the kth vertex	Interaction used at the $(k+1)$th vertex	Class of the diagram obtained at the $(k+1)$th vertex
A	1–2	A
	1–3 or 2–3	B
B	1–2	B
	1–3 or 2–3	B or C
C	1–2	C

happens to any of the diagrams obtained at the kth vertex when we add one interaction. This is given in Table I.

Let us consider a diagram of class B to which we add for instance an interaction 1–3. Then, depending on whether we choose vertices of the type (b), (f) or the type (d), (e) (see Fig. 1) we obtain a diagram of class B or C, respectively. In the case of the vertices (b), (f), the particle 3 remains at the left of the diagram and we obtain a diagram of class B. In the case of the vertex (d) or (e), this particle disappears from the diagram and we obtain a diagram of class C; however, whereas in the case $B \rightarrow B$ we can use any of the interactions 1–3 or 2–3, this is true for the case $B \rightarrow C$ only if both particles 1 and 2 are already present in the diagram at at the kth vertex. If only 1 (2) is present at this kth vertex, the k first interactions were 1–3 (2–3) and we may use only 2–3 (1–3) to destroy 3. Examples are given in Fig. 13.

To the diagrams of class B at the $(k+1)$th vertex corresponds the expression

$$\cdots(-\beta)^k \int dx^{(s-k-1)} G^{(123)}(x^{(s-k-2)} - x^{(s-k-1)})$$

$$\times \left\{ \frac{1}{k!} V_{12}{}^k [(\partial V_{13}/\partial x_1{}^{(s-k-1)}) D_{13}\right.$$

$$+ (\partial V_{23}/\partial x_2{}^{(s-k-1)}) D_{23}] + \sum_{p=0}^{k-1} \frac{1}{p!(k-p)!}$$

$$\times V_{12}{}^p (V_{13}+V_{23})^{k-p} [(\partial V_{12}/\partial x_1{}^{(s-k-1)}) D_{12}$$

$$\left. + (\partial V_{13}/\partial x_1{}^{(s-k-1)}) D_{13} + (\partial V_{23}/\partial x_2{}^{(s-k-1)}) D_{23}] \right\}$$

$$\times \exp[-\beta H_0], \quad (12.11)$$

where the first term corresponds to the diagrams of class B obtained from diagrams which were of class A at the kth vertex and the second from diagrams which were already of class B at the kth vertex.

Equation (12.11) can be rewritten as

$$\cdots(-\beta)^{k+1}\exp[-\beta H_0]$$
$$\times\int dx^{(s-k-1)}G^{(123)}(x^{(s-k-2)}-x^{(s-k-1)})$$
$$\times\Big\{\frac{1}{k!}V_{12}{}^{k}(\sum_{t=1}^{3}v_t\cdot\partial/\partial x_t{}^{(s-k-1)})(V_{13}+V_{23})$$
$$\times\sum_{p=1}^{k}\frac{1}{p!(k-p+1)!}(V_{13}+V_{23})^{k-p+1}$$
$$\times(\sum_{t=1}^{3}v_t\cdot\partial/\partial x_t{}^{(s-k-1)})V_{12}{}^{p}$$
$$+\sum_{p=0}^{k-1}\frac{1}{p!(k-p-1)!}V_{12}{}^{p}(\sum_{t=1}^{3}v_t\cdot\partial/\partial x_t{}^{(s-k-1)})$$
$$\times(V_{13}+V_{23})^{k-p-1}\Big\}$$
$$=\cdots(-\beta)^{k+1}\exp[-\beta H_0]\int dx^{(s-k-1)}$$
$$\times G^{(123)}(x^{(s-k-2)}-x^{(s-k-1)})(\sum_{t=1}^{3}v_t\cdot\partial/\partial x_t{}^{(s-k-1)})$$
$$\times[\sum_{p=0}^{k}\frac{1}{p!(k-p+1)!}V_{12}{}^{p}(V_{13}+V_{23})^{k-p+1}] \quad (12.12)$$

which, after performing the integrations in the usual way, gives (12.9) for $k\to k+1$.

We still have to consider the diagrams which are of class C at the $(k+1)$th vertex. As we have seen, some conditions must be taken into account when these diagrams are obtained from diagrams which were of class B at the kth vertex. We can do this in the following way: use both interactions 1–3 and 2–3 at the $(k+1)$th vertex and subtract from the diagrams obtained in this way the diagrams obtained by using an interaction 1–3 (2–3) for a diagram for which the k first interactions were 1–3 (2–3) only. The expression for the diagrams of class C at the $(k+1)$th vertex will then be

$$\cdots(-\beta)^{k}\int dx^{(s-1-k)}G^{(123)}(x^{(s-2-k)}-x^{(s-1-k)})$$
$$\times\Big\{\sum_{p=0}^{k-1}\frac{1}{p!(k-p)!}V_{12}{}^{p}(V_{13}+V_{23})^{k-p}$$
$$\times[(\partial V_{13}/\partial x_1{}^{(s-k-1)})D_{13}+(\partial V_{23}/\partial x_2{}^{(s-k-1)})D_{23}]$$
$$-(1/k!)[V_{13}{}^{k}(\partial V_{13}/\partial x_1{}^{(s-k-1)})D_{13}$$
$$+V_{23}{}^{k}(\partial V_{23}/\partial x_2{}^{(s-k-1)})D_{23}]$$
$$+\sum_{p=0}^{k-2}\frac{1}{p!(k-p)!}V_{12}{}^{p}[(V_{13}+V_{23})^{k-p}-V_{13}{}^{k-p}$$
$$-V_{23}{}^{k-p}]\times(\partial V_{12}/\partial x_1{}^{(s-k-1)})D_{12}\Big\}\exp[-\beta H_0]$$
$$=\cdots(-\beta)^{k+1}\exp[-\beta H_0]\int dx^{(s-k-1)}$$
$$\times G^{(123)}(x^{(s-k-2)}-x^{(s-k-1)})$$
$$\times(\sum_{t=1}^{3}v_t\cdot\partial/\partial x_t{}^{(s-k-1)})\Big\{\sum_{p=0}^{k-1}\frac{1}{p!(k-p+1)!}$$
$$\times V_{12}{}^{p}[(V_{13}+V_{23})^{k-p+1}-V_{13}{}^{k-p+1}-V_{23}{}^{k-p+1}]\Big\}$$
$$+\cdots(-\beta)^{k+1}\exp[-\beta H_0]\int dx^{(s-k+1)}$$
$$\times G^{(123)}(x^{(s-k-2)}-x^{(s-k-1)})\Big\{\sum_{p=1}^{k-1}\frac{1}{p!(k-p+1)!}V_{12}{}^{p}$$
$$\times(\sum_{t=1}^{3}v_t\cdot\partial/\partial x_t{}^{(s-k-1)})$$
$$\times[V_{13}{}^{k-p+1}+V_{23}{}^{k-p+1}]\Big\}. \quad (12.13)$$

The second term in the rhs of (12.13) vanishes. Indeed, as we deal with diagrams of class C, particle 3 will no longer appear after the $(k+1)$th vertex. Therefore, in (12.11), we could have integrated over all $dx_3{}^{(i)}$, $1\leqslant i\leqslant s-k-2$.

The second term in the rhs of (12.13) can be written

$$\int dx_1{}^{(s-k-1)}dx_2{}^{(s-k-1)}dx_3{}^{(s-k-1)}G^{(12)}(x^{(s-k-2)}-x^{(s-k-1)})$$
$$+\sum_{p=1}^{k-1}\frac{1}{p!(k-p+1)!}V_{12}{}^{p}(\sum_{t=1}^{3}v_t\cdot\partial/\partial x_t{}^{(s-k-1)})$$
$$\times(V_{13}{}^{k-p+1}+V_{23}{}^{k-p+1}). \quad (12.14)$$

Let us for instance consider the first term and take as integration variables

$$R=[x_1{}^{(s-k-1)}+x_2{}^{(s-k-1)}+x_3{}^{(s-k-1)}]/3,$$
$$x_{12}=x_1{}^{(s-k-1)}-x_2{}^{(s-k-1)};\quad x_{13}=x_1{}^{(s-k-1)}-x_3{}^{(s-k-1)}.$$

Integrating over the center of mass, we obtain

$$\int dx_{12}G^{(12)}(x_{12}{}^{(s-k-2)}-x_{12})\sum_{p=1}^{k-1}\frac{1}{p!(k-p+1)!}V_{12}{}^{p}$$
$$\times\int dx_{13}(v_{13}\cdot\partial/\partial x_{13})V_{13}{}^{k-p+1}=0. \quad (12.15)$$

The first term in the rhs of (12.15) can be dealt with in the usual manner and gives simply (12.10) for $k\to k+1$.

We can go on with this procedure; however, we are interested in the diagrams with s vertices which contribute to the Fourier coefficient describing a correlation between two particles 1 and 2. This means that at the sth vertex, we only have to consider the diagrams of class C. Therefore, we obtain as our net result an

expression similar to (10.20):

$$[\rho_{(1)}{}^{(s)}]_{C^2} \to (\pi\beta^{-1})^{3N/2}N\Omega^{-2}(-\beta)^s \exp[-\beta H_0]$$
$$\times\langle l|G^{(12)}|l\rangle \int dx_1dx_2dx_3 \exp(-ilx_{12})$$
$$\times(\sum_{t=1}^{3} v_t\cdot\partial/\partial x_t)\Big\{\sum_{p=0}^{s-2}\frac{1}{p!(s-p)!}V_{12}{}^p[(V_{13}+V_{23})^{s-p} - V_{13}{}^{s-p}-V_{23}{}^{s-p}]\Big\}$$
$$=C(\pi\beta^{-1})^{3N/2}(-\beta)^s \exp[-\beta H_0]$$
$$\times\int dx_{12}\exp(-ilx_{12})\Big\{\sum_{p=0}^{s-2}\frac{1}{p!(s-p)!}V_{12}{}^p$$
$$\times\int dx_3[(V_{13}+V_{23})^{s-p}-V_{13}{}^{s-p}-V_{23}{}^{s-p}]\Big\}$$
$$=C(\pi\beta^{-1})^{3N/2}(-\beta)^s \exp[-\beta H_0]$$
$$\times\int dx_{12}\exp(-ilx_{12})\Big\{\sum_{p=0}^{s-2}\frac{1}{p!}V_{12}{}^p$$
$$\times\int dx_3\Big[\sum_{q=1}^{s-p-1}\frac{1}{q!(s-p-q)!}V_{13}{}^qV_{23}{}^{s-p-q}\Big]\Big\} \quad (12.16)$$

in complete agreement with (8.13).

In order to have a complete H theorem at order C^2, we still have to show that the triple correlation 1–2–3 reaches the correct value. This can be done in the same way. In this case, particle 3 is no longer a dummy particle and therefore we must exclude all diagrams of class C. At the sth vertex, we have only diagrams of class B with the condition that the three particles 1–2–3 are present. Such a condition can be taken into account in a way similar to that used previously when building diagrams of class C from diagrams of class B.

We shall not establish the H theorem at higher orders in C. All characteristic features have now been introduced. For each of the particles $3\cdots k-1$, one must define the class B_i and C_i. If we consider for instance the contribution to the pair correlation at order C^k, we have $(k-1)$ dummy particles and the diagrams we have to consider at the sth vertex are of the type $C_3C_4\cdots C_{k-1}$. Therefore, from each of those particles start at least two bonds. Moreover particles 1 and 2 must have interacted at least with one of the dummy particles in order to be at the left of the diagrams. Therefore they are connected to the other particles in the cluster diagrams.

To prove the H theorem, we should still show that diagrams which correspond to cluster diagrams with an articulation point give vanishing contributions. Let us consider the physical meaning of such diagrams. All the dummy particles which are in the appending part of the diagram have interacted among themselves and with only *one* of the particles which form the main part of the diagram. This part of the diagram plays no role in the building of the correlation 1–2. It essentially corresponds to a scattering process. Now, we have seen that such scattering processes are effective in the establishment of the correct velocity distribution function but become ineffective once this is achieved, which is precisely the situation we are dealing with. Therefore, we may really expect that such diagrams will give a vanishing contribution and that the only diagrams which give a nonvanishing contribution are those where each dummy particle plays a role in the building of the correlation. Such diagrams precisely correspond to the irreducible cluster diagrams. In fact, each of these cluster diagrams corresponds to several creation fragments, this being due to the various possible chronological orders of the interactions involved.

13. CONCLUSIONS

We have seen that the equations which describe the evolution of the system are such that all physical quantities which are functions of a finite number of degrees of freedom will reach the correct equilibrium value after a long time. This is a remarkable extension of Boltzmann's H theorem. Whereas Boltzmann's H theorem is concerned only with the reduced velocity distribution function f_1, our proof takes also into account the correlations between the particles introduced by their mutual interaction energy. Therefore our proof is valid for space-dependent quantities too. We want to stress the fact that the proof given in the foregoing is based upon very few hypotheses.

These hypotheses concern the class of initial distribution functions we consider. Two aspects are involved: first, the dependence with respect to the number of particles and the volume; secondly, the dependence with respect to the coupling constant λ. The first one is in fact all that is needed to establish the general H theorem. Indeed, if we modify the λ dependence in the initial conditions, we shall modify the order with respect to λ of all the diagrams which do not involve $\rho_0(t)$; however, their asymptotic properties will not be modified by this procedure. Therefore, the *only* hypothesis involved in the proof of the general H theorem is the dependence with respect to N and Ω of the distribution function. This hypothesis has a very simple physical meaning: extensive and intensive properties of the system in the thermodynamical sense may be defined from the initial state. This indeed corresponds to the situation encountered in a large number of physical systems. This hypothesis is far less restrictive than those used in equilibrium theory.[10] There, in order to obtain the equilibrium distribution for functions of a finite number of degrees of freedom, one has to specify the distribution function for the entire system

[10] A. Khinchin, *Mathematical Foundations of Statistical Mechanics* (Dover Publications, New York, 1949).

(microcanonical distribution). Although our results are equivalent with those of the equilibrium theory, we never need such a specification of the complete distribution function.

In fact, the behavior of this function is always described by the Liouville equation; however, no matter how complicated this behavior may be, whenever intensive properties in the thermodynamical sense may be defined, our results will be valid.

ACKNOWLEDGMENTS

We express our profound thanks to Professor I. Prigogine for suggesting this work and his constant help during it.

APPENDIX—ASYMPTOTIC TIME INTEGRATIONS

1. Resolvent Operator

Let us give here a method which allows a derivation of the theorems stated in Sec. 4 in a very compact and elegant way.

We start from the Liouville equation

$$i\partial\rho/\partial t = L\rho = (L_0+\lambda\delta L)\rho. \tag{A1}$$

We define a resolvent operator[11] $(L-z)^{-1}$, which is a function of the complex variable z. It is known (see Stone[12]) that this resolvent is bounded for nonreal z. The formal solution of (A1) may obviously be written as

$$\rho(t) = -(2\pi i)^{-1}\oint_C dz \frac{e^{-izt}}{L-z}\rho(0), \tag{A2}$$

where the contour C is shown in Fig. 14. We may also introduce a resolvent $(L_0-z)^{-1}$ for the unperturbed Liouville operator L_0. On using the identity

$$A^{-1}-B^{-1} = A^{-1}(B-A)B^{-1}, \tag{A3}$$

we may write

$$(L-z)^{-1} = (L_0-z)^{-1} - \lambda(L_0-z)^{-1}\delta L(L-z)^{-1}, \tag{A4}$$

or, by an iterative procedure (assuming that the series converges),

$$(L-z)^{-1} = \sum_{n=0}^{\infty}(-\lambda)^n(L_0-z)^{-1}[\delta L(L_0-z)^{-1}]^n. \tag{A5}$$

If we express our formal solution, given by (A2) and (A5), in the Fourier representation of the N particle system, we obtain

$$\rho_{\{k\}}(\{v\},t) = -(2\pi i)^{-1}\oint dz\exp(-izt)\sum_{\{k'\}}\sum_{n=0}^{\infty}(-\lambda)^n \times\langle\{k\}|(L_0-z)^{-1}[\delta L(L_0-z)^{-1}]^n|\{k'\}\rangle \times\rho_{\{k'\}}(\{v\},0). \tag{A6}$$

[11] L. Van Hove, Physica 21, 901 (1955).

[12] M. H. Stone, *Linear Transformation in Hilbert Space* (American Mathematical Society, New York, 1932).

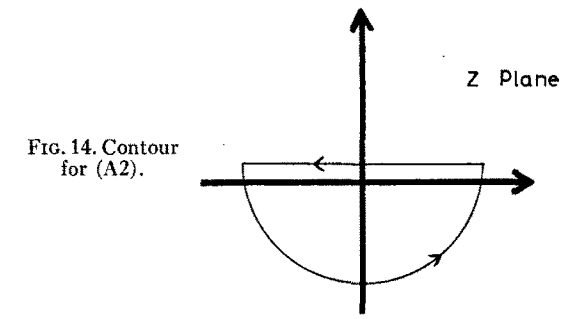


FIG. 14. Contour for (A2).

We notice that in Fourier space, the resolvent of the unperturbed system is diagonal

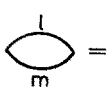
$$\langle\{k\}|[L_0-z]^{-1}|\{k'\}\rangle = [\textstyle\sum_j k_jv_j-z]^{-1}\delta^{Kr}{}_{\{k\},\{k'\}}. \tag{A7}$$

We may thus associate the same diagrams to Eq. (A6) as we did for the iterative solution of (2.6), the only difference being that to each state $\{k\}$ (final, intermediate or initial) we associate a "time independent propagator" $[\sum_j k_jv_j-z]^{-1}$ instead of the oscillating exponentials $\exp[i\sum_j k_jv_j(t_n-t_{n-1})]$.

The analysis of the asymptotic behavior for long times of the different contributions involved in (A6) will give us a simple and rigorous proof of the theorems of Sec. 4. Let us first study in great detail two particular examples.

2. Cycle and Free Propagation

(a) The contribution to (A6) corresponding to a cycle is



$$= -(2\pi i)^{-1}\oint dz \times\exp(-izt)\{\lambda^2\sum_{\{k\}} z^{-1}\langle 0|\delta L_{lm}|\{k\}\rangle \times[\textstyle\sum_j k_jv_j-z]^{-1}\langle\{k\}|\delta L_{lm}|0\rangle z^{-1}\}\rho_0(\{v\},0). \tag{A8}$$

Let us consider the expression

$$\psi(z,\{v\}) = \sum_{\{k\}}\langle 0|\delta L_{lm}|\{k\}\rangle[\textstyle\sum_j k_jv_j-z]^{-1} \times\langle\{k\}|\delta L_{lm}|0\rangle. \tag{A9}$$

On using (2.7) and replacing the sum over $\{k\}$ by an integral, we immediately obtain

$$\psi(z,\{v\}) = -(8\pi^3\Omega)^{-1}\int d^3\mathbf{k}V_k\mathbf{k}\cdot\mathbf{D}_{lm} \times[\mathbf{k}\cdot\mathbf{v}_{lm}-z]^{-1}V_{-k}\mathbf{k}\cdot\mathbf{D}_{lm}. \tag{A10}$$

We choose a system of cylindrical coordinates for $\mathbf{k}$, with polar axis directed along $\mathbf{v}_{lm}$; we may then bring

this integral to the general form

$$\varphi(z)=\int_{-\infty}^{\infty} d\omega \frac{f(\omega)}{\omega-z}, \tag{A11}$$

which is known as a Cauchy integral[13]; one of its fundamental properties is given by the following theorem: if $f(\omega)$ satisfies the Lipschitz condition

$$|f(\omega_1)-f(\omega_2)| \leqslant C|\omega_1-\omega_2|^{\alpha}, \quad (0\leqslant\alpha<1), \tag{A12}$$

$\varphi(z)$ is an analytic function of z in the upper and in the lower half-plane, except for a finite discontinuity along the real axis.

We shall always assume that the integrand of (A10) satisfies the required conditions and we shall denote by $\psi^+(z,\{v\})$ the integral calculated for $\mathrm{Im}z>0$.

We shall also suppose that $\psi^+(z,\{v\})$ has an analytical continuation in the lower plane; this continuation is of course *not* identical to the function $\psi^-(z,\{v\})$ defined by (A10) when $\mathrm{Im}z<0$; on the contrary, it will have poles in this part of the complex plane; these poles will be situated at points such that $\mathrm{Im}z \simeq \mathbf{v}\cdot\bar{\boldsymbol{\kappa}}$ where $\bar{\kappa}^{-1}$ is some characteristic length, of the order of the range of the forces $V(r)$.[14]

For $t>0$, the integral on the semicircle at infinity gives no contribution, and we may write for (A8)

$$\underset{m}{\overset{l}{\bigcirc}} = -(2\pi i)^{-1}\lambda^2 \oint dz z^{-2} \times \exp(-izt)\psi^+(z,\{v\})\rho_0(\{v\},0), \tag{A13}$$

where we use for $\psi^+(z)$ in the lower half-plane the analytical continuation of (A10) calculated for $\mathrm{Im}z>0$.

We may now perform the z integration, applying the residue theorem

$$(2\pi i)^{-1}\oint f(z)dz=\sum(\text{Res } f(z) \text{ inside the contour}). \tag{A14}$$

We get, in this case, a second-order pole at $z=0$ and poles arising from the function $\psi^+(z,\{v\})$ at points in the lower half-plane

$$\underset{m}{\overset{l}{\bigcirc}} = -\lambda^2\{-it\psi^+(0,\{v\})+\psi'^+(0,\{v\}) + \sum_i z_i^{-2}\exp(-iz_it)[\mathrm{Res}\psi^+(z)]_{z=z_i}\}. \tag{A15}$$

Let us point out that formula (A15) is still exact; no asymptotic estimations have been made. If we now use the fact that the poles z_i of $\psi^+(z,\{v\})$ are such that

$$\mathrm{Im}z_i \simeq \bar{\kappa}\mathbf{v} \tag{A16}$$

for times t much larger than the duration of a collision, we have

$$(\mathrm{Im}z_i)t \simeq \bar{\kappa}\cdot\mathbf{v}t \gg 1, \tag{A17}$$

and we are thus left with a contribution which grows asymptotically as t.

More precisely,

$$\underset{m}{\overset{l}{\bigcirc}} = -\lambda^2 it\psi^+(0,\{v\}) \tag{A18}$$

$$=\lambda^2(8\pi^3\Omega)^{-1}t\int d^3\mathbf{k}|V_k|^2\mathbf{k}\cdot\mathbf{D}_{lm}[\pi\delta_-(\mathbf{k}\cdot\mathbf{v}_{lm})] \times\mathbf{k}\cdot\mathbf{D}_{lm}\rho_0(\{v\},0) \tag{A19}$$

using well-known formulas for Cauchy integrals [see footnote reference 13 and (A26)]. This is exactly the result which was obtained in footnote reference 1 by studying the asymptotic behavior of oscillating exponentials, which we never encounter in this method. Let us point out that the advantage of the proof presented here is essentially related to the fact that we first performed (in a formal way) the summation over the $\mathbf{k}$ vector (getting an integral of the Cauchy type) and *then* evaluated the z integral; had we calculated the z integral first, we would have been left with the oscillating factors.

(b) Let us consider the case of the "free propagation" of a correlation

$$\frac{\alpha}{\beta} = -(2\pi i)^{-1}\oint dz \exp(-izt)[\mathbf{k}\mathbf{v}_{\alpha\beta}-z]^{-1} \times\rho_{\mathbf{k}_\alpha,-\mathbf{k}_\beta}(\{v\},0). \tag{A20}$$

Clearly, in this form, there is no $\mathbf{k}$ integration; however, if we realize that we are actually interested in the distribution function in phase space, i.e., in

$$f^{(0)}(\mathbf{x}_{\alpha\beta};\{\mathbf{v}\};t)\sim-(2\pi i)^{-1}\oint dz\exp(-izt) \times\sum_{\mathbf{k}}\exp(i\mathbf{k}\mathbf{x}_{\alpha\beta})[\mathbf{k}\mathbf{v}_{\alpha\beta}-z]^{-1}\rho_{\mathbf{k}_\alpha,-\mathbf{k}_\beta}(\{\mathbf{v}\},0), \tag{A21}$$

it is tempting to interpret the $\mathbf{k}$ integral as we did in the case of the cycle; but this would now imply assumptions about the locations of the poles of $\rho_{\mathbf{k}_\alpha,-\mathbf{k}_\beta}$ [see (A16)] and would be a much too restrictive choice of our initial conditions.

In fact, *we want to study the reduced distribution functions of our system for small distances* $\mathbf{x}_{\alpha\beta}$ *in the limit of long times. But we want to be able to study initial conditions in which the range of correlations is arbitrary.* (For the other restriction, see the discussion in Sec. 13.) We are thus obliged in this case to treat the z integral exactly and then to perform the summation over $\mathbf{k}$:

[13] N. I. Muskhelishvili, *Singular Integral Equations* (Noordhoff-Groningen, 1953).

[14] The reader may verify these statements by evaluating the the integral (A10) with a typical potential; for instance, with $V(r)=\exp[-\kappa r]$, whose Fourier transform is $V_k=8\pi\kappa/(\kappa^2+k^2)^2$.

we then obtain

$$f^{(0)}(\mathbf{x}_{\alpha\beta};\{\mathbf{v}\};t)\sim\sum_{\mathbf{k}}\exp[i\mathbf{k}(\mathbf{x}_{\alpha\beta}-\mathbf{v}_{\alpha\beta}t)]\times\rho_{\mathbf{k}_\alpha,-\mathbf{k}_\beta}(\{\mathbf{v}\},0), \quad \text{(A22)}$$

which gives an exact description of the free propagation of the two particles involved.

It is now clear that if we want to be consistent, in any diagram where we have one particle which propagates through the whole time interval $0\to t$, we shall have to treat it exactly. This is why we have used the "subtraction" procedure in Sec. 4 before giving the general theorems on time integration.

The easiest way to make this subtraction in the resolvent method (neglecting here the problems of commutations which have been discussed in footnote reference 2) is to use a change of variables in (A6); we put

$$z'=z-\sum{}'\,\mathbf{k}_\alpha\mathbf{v}_\alpha, \quad \text{(A23)}$$

where the summation extends over all particles α which propagate through the whole diagram and where $\mathbf{k}_\alpha$ is the total momentum of the disconnected part which involves this particle α; (A6) then becomes

$$\rho_{\{\mathbf{k}\}}(\{\mathbf{v}\},t)=-(2\pi i)^{-1}\exp[-i\sum{}'\,\mathbf{k}_\alpha\mathbf{v}_\alpha t]\times\sum_{\{\mathbf{k}'\}}\sum_{n=0}^{\infty}(-\lambda)^n\oint\exp(-iz't)dz'\times\langle\{\mathbf{k}\}|(L_0'-z')^{-1}[\delta L(L_0'-z')^{-1}]^n|\{\mathbf{k}'\}\rangle\times\rho_{\{\mathbf{k}'\}}(\{\mathbf{v}\},0), \quad \text{(A24)}$$

with

$$L_0'=L_0-\sum{}'\,\mathbf{k}_\alpha\mathbf{v}_\alpha. \quad \text{(A25)}$$

3. General Theorems

We can now generalize the argument of the preceding section to the most complicated cases; however, as we have learned how to deal with propagation diagrams and how to reduce them by (A23) to a basic structure (see Sec. 4) without propagation, we shall only consider the latter case.

We follow the general procedure:

(1) Write down the contribution of a given diagram in the resolvent formalism.

(2) Evaluate then all possible summations (in a formal way) over $\mathbf{k}$ vectors (or eventually over $\mathbf{v}$ vectors) in order to get an integral of the Cauchy type $\psi^+(z)$.

We always assume that these generalized Cauchy integrals may be continued analytically in the lower half-plane but their poles z_i satisfy (A16).

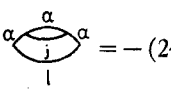
(3) Then perform the z integration, keeping only the contributions coming from the poles on the real axis [in fact at $z=0$ when we use (A24)], which have not been eliminated by the Cauchy integrations.

(4) Interpret $\psi^+(0)$ applying the well-known representation of the $\delta_-(x)$ function

$$\pi\delta_-(x)=1/i(x-i\epsilon). \quad \text{(A26)}$$

We can then readily prove our general theorems by induction; however we shall only give here typical examples:

(A) A single diagonal diagram gives an asymptotic contribution of maximum order t. Consider the following case:



$$=-(2\pi i)^{-1}\oint dz\exp(-izt)\Omega^{-4}\times\sum_{\mathbf{k}}\sum_{\mathbf{l}}z^{-1}iV_{\mathbf{k}}\mathbf{k}\cdot\mathbf{D}_{\alpha l}[\mathbf{k}\cdot\mathbf{v}_{\alpha l}-z]^{-1}iV_{\mathbf{l}}\mathbf{l}\cdot\mathbf{D}_{\alpha j}\times[\mathbf{k}\cdot\mathbf{v}_{\alpha l}+\mathbf{l}\cdot\mathbf{v}_{\alpha j}-z]^{-1}(-i)V_{-\mathbf{l}}\mathbf{l}\cdot D_{\alpha j}\times[\mathbf{k}\mathbf{v}_{\alpha l}-z]^{-1}(-i)V_{-\mathbf{k}}\mathbf{k}\cdot\mathbf{D}_{\alpha l}z^{-1}\rho_0(\{v\},0). \quad \text{(A27)}$$

Performing formally the summations over $\mathbf{k}$ and $\mathbf{l}$, we are left with a second-order pole at $z=0$ and we thus get, in the limit of long times, a contribution of order t; we see clearly in this example the compactness of the method compared to the study of the asymptotic behavior of oscillating exponentials[1]; however, the latter demonstration is more intuitive and requires a simpler mathematical technique.

The generalization to a diagonal fragment $[O(t)]$ or to a succession of diagonal fragments is trivial; whenever we add a diagonal fragment we get a new z^{-1} factor and thus a supplementary t factor:

(B) A succession of m diagonal fragments gives an asymptotic contribution of order t^m.

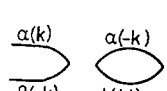
(C) The destruction of a correlation followed by m successive diagonal fragments gives asymptotically a contribution of maximum order t^m

For instance,

$$=-(2\pi i)^{-1}\oint dz\times\exp(-izt)\Omega^{-3}\sum_{\mathbf{k}}\sum_{\mathbf{l}}z^{-1}iV_{\mathbf{k}}\mathbf{k}\cdot\mathbf{D}_{\alpha l}\times[\mathbf{k}\cdot\mathbf{v}_{\alpha l}-z]^{-1}(-i)V_{-\mathbf{k}}\mathbf{k}\cdot\mathbf{D}_{\alpha l}z^{-1}iV_{\mathbf{l}}\mathbf{l}\cdot\mathbf{D}_{\alpha n}\times[\mathbf{l}\cdot\mathbf{v}_{\alpha n}-z]^{-1}\rho_{\mathbf{l}_\alpha,-\mathbf{l}_n}. \quad \text{(A28)}$$

All propagators except the two poles at $z=0$ may be included in the generalized Cauchy integral obtained by summing over $\mathbf{k}$ and $\mathbf{l}$. There remains a double pole at $z=0$ which gives a t factor. The proof for any destruction fragment followed by n diagonal fragments runs along the same lines.

(D) The creation of a correlation preceded by m diagonal transitions gives asymptotically a contribution of order t^m. Consider the following diagram:



$$=-(2\pi i)^{-1}\lambda^3\oint dz\exp(-izt)\times\Omega^{-3}\sum_{\mathbf{k}'}[\mathbf{k}\cdot\mathbf{v}_{\alpha\beta}-z]^{-1}iV_{\mathbf{k}}\mathbf{k}\cdot\mathbf{D}_{\alpha\beta}z^{-1}iV_{\mathbf{k}'}\mathbf{k}'\cdot\mathbf{D}_{\alpha l}\times[\mathbf{k}'\cdot\mathbf{v}_{\alpha l}-z]^{-1}(-i)V_{\mathbf{k}'}\mathbf{k}'\cdot\mathbf{D}_{\alpha l}z^{-1}\rho_0(\{\mathbf{v}\},0). \quad \text{(A29)}$$

As long as we remain in Fourier representation, we have no summation which allows us to bring the first propagator in an integral of the Cauchy type; however, as we have already noticed earlier [see (A21)], we are interested in distribution functions in ordinary space. We thus must multiply (A28) by $\exp(i\mathbf{k}\cdot\mathbf{x}_{\alpha\beta})$ and sum over $\mathbf{k}$. If we are only interested in small values of $\mathbf{x}_{\alpha\beta}$ (i.e., of the order of the molecular correlation length), conditions (A12) and (A16) are both satisfied and we may include the propagator in a Cauchy integral over $\mathbf{k}$. The double pole at $z=0$ remains and accordingly we get a t factor.

(E) Irreducible destruction-creation fragment: the physical meaning of (A28) and (A29) is clear. As explained in the text, a destruction (a creation) fragment is an almost instantaneous event which takes place at time $t'=0$ ($t'=t$). It is then clear, and this could be confirmed by a detailed calculation, that a diagram such as those given in Fig. 5 could not possibly give any time growing contribution. The same property may also be verified for any destruction diagram which corresponds to initial and final state with $\{k_i\}\neq 0$.

Combining the proofs (A)–(E), we immediately obtain our basic theorems I and II of Sec. 4.

Note added in proof. One of us (P.R.) has recently generalized the method used in this (as well as in the preceding) paper to obtain an H theorem valid in *both* cases to all powers of the concentration or the coupling constant. This method applies as well to the quantum case. A preliminary paper has been presented to publication to the Phys. Rev. Letters. On the other hand, the proof that the correlations reach their equilibrium value once the velocity distribution is the equilibrium one, can be greatly simplified, as has been shown by one of us (F.A.).

We also want to make the following remarks about asymptotic time integration: the procedure to be used depends, in a sense, upon the type of quantities whose time evolution is considered. One may be interested in the time evolution of phase correlations in Fourier space (irrespective of the distance between the particles), in which case the asymptotic time integration cannot be applied to the last creation fragment. Another limiting situation corresponds to the time evolution of quantities which drop out to zero at large intermolecular distances (as do all thermodynamic properties, for example). We then have an integration over the whole set of Fourier components. The oscillating sum

$$\sum_{\{\mathbf{k}\}} \rho'_{\{\mathbf{k}\}} \exp[i \sum_j \mathbf{k}_j\cdot(\mathbf{r}_j-\mathbf{v}_j t)]$$

decays to zero after times of the order of a collision time (for molecular correlation). In a sense, whenever one wants to go beyond the usual Boltzmann kind of equation, the kinetics of the approach to equilibrium depend on some general characteristics of the initial state (for example on the range of the correlations), but in all cases, for sufficiently large times, complete statistical equilibrium is reached. These problems will be considered in detail in a separate publication.

On the General Theory of the Approach to Equilibrium. III. Inhomogeneous Systems*

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We find the evolution equation for a singlet distribution function in a fluid containing macroscopic inhomogeneities. The equation, a generalization of the Boltzmann equation, derived from the Liouville equation, may be written formally to any order in either concentration or strength of interaction. We find f_1 to be a functional only of itself and other f_1's. We then show that initially present correlations are destroyed during the same relaxation time as in homogeneous systems. We can then write formally to any order the equation for a reduced s-particle distribution function f_s, which proves to be a functional of a product of f_1's, all the time dependence of the f_s being lodged in the f_1's for times greater than the relaxation time.

1. INTRODUCTION

RECENTLY Prigogine and co-workers have presented a perturbation method of solving the Liouville equation in the limit of infinite volume and number of particles, but finite concentration.[1–4] This method utilizes a diagram technique for evaluating the magnitudes of the contributions to various Fourier components of the distribution function. With these techniques, Prigogine and Henin[5] have studied the approach to equilibrium in solids, and Henin, Résibois, and Andrews[4] the approach to equilibrium in homogeneous fluids. This latter work shows that all the classical results of equilibrium statistical mechanics may be considered as the natural outcome of the irreversible approach to equilibrium of a dynamical system. This is so to any order in any selected perturbation parameter.

In this paper we wish to consider systems with a macroscopic inhomogeneity of the type discussed by Prigogine and Balescu.[2] We study the time evolution of reduced distribution functions by the method given in footnote reference 4, and we learn that the approach to equilibrium of these systems may be considered a stepwise process characterized by the times $t_h \gg t_r \gg t_0$, where t_h is characteristic of the hydrodynamical relaxation time, t_r of the molecular relaxation time, and t_0 of the collision time. We have then derived formally and given explicit expression to the ideas presented by Bogoliubov.[6]

2. EVOLUTION OF THE SINGLET DISTRIBUTION FUNCTION

The singlet or reduced one-particle distribution function is defined in the usual manner[1–3] by

$$f_1(\mathbf{x}_\alpha,\mathbf{v}_\alpha,t)=C\{\rho_0(\mathbf{v}_\alpha,t) +\Omega^{-1}\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot(\mathbf{x}_\alpha-\mathbf{v}_\alpha t)]\rho_{\mathbf{k}}(\mathbf{v}_\alpha,t)\} \quad (2.1)$$

with the equation of change

$$\frac{\partial f_1(\alpha)}{\partial t}+\mathbf{v}_\alpha\cdot\frac{\partial f_1(\alpha)}{\partial \mathbf{x}_\alpha} =C\frac{\partial \rho_0(\alpha)}{\partial t}+C\Omega^{-1}\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot(\mathbf{x}_\alpha-\mathbf{v}_\alpha t)]\frac{\partial \rho_{\mathbf{k}}(\alpha)}{\partial t}. \quad (2.2)$$

Throughout this paper for a general wave vector $\mathbf{n}$ we shall use the notation $\mathbf{k}$ for macroscopic, i.e., small wave vectors and $\mathbf{l}$ for molecular, i.e., large, wave vectors.[2]

We shall study the rhs of Eq. (2.2) when the time derivatives are caused by a particular diagonal $\rho_0 \to \rho_0$ skeleton operator, $X_{\eta\mu}$, whose diagram has η vertices and involves μ different particles ($\mu \leq \eta$). $X_{\eta\mu}$ will have arisen as one of the operators effective to the order of perturbation being taken (i.e., $\lambda^\eta t$ in weakly coupled systems, $C^{\mu-1}t$ in dilute gases, or a combination of these). Since we study the evolution of $f_1(\mathbf{x}_\alpha,\mathbf{v}_\alpha,t)$, the last vertex on the left of $X_{\eta\mu}$ "destroys" particle α. There must be in $X_{\eta\mu}$ both a creation and a destruction vertex for each of the μ particles. In addition to $X_{\eta\mu}$, we must consider the entire set of "pseudodiagonal" operators formed by adding to the left of $X_{\eta\mu}$ a weak correlation line (with small propagation vector characteristic of macroscopic inhomogeneities) for particle α and going to the right any combination of weak lines coming from creation vertices for any particles being created.

This set of operators contains $X_{\eta\mu}$ acting on

$$\prod_{i=1}^{\mu}\rho_0(\mathbf{v}_i);$$

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[1] I. Prigogine and R. Balescu (I and II), Physica **25**, 281, 302 (1959).

[2] I. Prigogine and R. Balescu (III), Physica (to be published).

[3] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience Publishers, Inc., New York, to appear in 1960).

[4] F. Henin, P. Résibois, and F. Andrews, J. Math. Phys. **2**, 68 (1960), preceding paper.

[5] I. Prigogine and F. Henin, J. Math. Phys. **1**, 349 (1960).

[6] N. N. Bogoliubov, J. Phys. U.S.S.R. **10**, 265 (1946). See also Mark Kac with G. E. Uhlenbeck, *Probability and Related Topics in Physical Science* (Interscience Publishers, Inc., New York, 1959), pp. 195–199.

then the μ different terms

$$X_{\eta\mu} \prod_{i=1,\neq\zeta}^{\mu} \rho_0(\mathbf{v}_i)\rho_1(\zeta),$$

where ζ is the particle whose weak propagation line goes to the right, the term also containing a weak α line going to the left; then the $\mu(\mu-1)$ different terms

$$X_{\eta\mu} \prod_{i=1,\neq\{\zeta\}}^{\mu} \rho_0(\mathbf{v}_i) \prod_{j=\{\zeta\}} \rho_1(j),$$

where $\{\zeta\}$ is the set of two particles whose weak propagation lines go to the right, the term of course also having a weak α line to the left; $\cdots$; finally the term

$$X_{\eta\mu} \prod_{j=1}^{\mu} \rho_1(j).$$

On substituting this set of terms into the rhs of Eq. (2.2), the $\exp(-i\mathbf{k}\cdot\mathbf{v}_\alpha t)$ in (2.2) cancels the exponential representing the weak α lines on the left of the operator terms. The $\exp(i\mathbf{k}\cdot\mathbf{x}_\alpha)$ commutes with the entire operator, since it merely acts in velocity space. By conservation of wave vectors, this $\mathbf{k}$ may be equated to the sum of the wave vectors of the weak propagation lines on the right, and in the limit of infinite volume may be considered an integral over new variables of the form

$$\int \prod_{\{\zeta\}} \{d\mathbf{k}_\zeta \rho_{\mathbf{k}_\zeta}(\zeta) \exp[i\mathbf{k}_\zeta\cdot(\mathbf{x}_\alpha-\mathbf{v}_\zeta t)]\}.$$

So the combination of all the operators in the previous paragraph gives the rhs of Eq. (2.2) the form (omitting for the moment the integrals over velocities of the μ particles $\neq\alpha$ necessary to reduce the distribution function to a singlet function):

$$X_{\eta\mu} \prod_{i=1}^{\mu} \rho_0(\mathbf{v}_i) + \sum_{\zeta} X_{\eta\mu} \prod_{i=1,\neq\zeta}^{\mu} \rho_0(\mathbf{v}_i) \int d\mathbf{k}_\zeta \rho_{\mathbf{k}_\zeta}(\zeta)$$

$$\times \exp[i\mathbf{k}_\zeta\cdot(\mathbf{x}_\alpha-\mathbf{v}_\zeta t)] + \sum_{\{\zeta\}} X_{\eta\mu} \prod_{i=1,\neq\{\zeta\}}^{\mu} \rho_0(\mathbf{v}_i)$$

$$\times \int \prod_{\{\zeta\}} \{d\mathbf{k}_\zeta \rho_{\mathbf{k}_\zeta}(\zeta) \exp[i\mathbf{k}_\zeta\cdot(\mathbf{x}_\alpha-\mathbf{v}_\zeta t)]\} + \cdots$$

$$+ X_{\eta\mu} \int \prod_{\zeta=1}^{\mu} \{d\mathbf{k}_\zeta \rho_{\mathbf{k}_\zeta}(\zeta) \exp[i\mathbf{k}_\zeta\cdot(\mathbf{x}_\alpha-\mathbf{v}_\zeta t)]\}. \quad (2.3)$$

Since from Eq. (2.1),

$$C^{-\mu} X_{\eta\mu} \prod_{i=1}^{\mu} f_1(\mathbf{x}_\alpha,\mathbf{v}_i,t)$$

$$= X_{\eta\mu} \prod_{i=1}^{\mu} \{\rho_0(\mathbf{v}_i) + \int d\mathbf{k}\rho_{\mathbf{k}}(\alpha i) \exp[i\mathbf{k}\cdot(\mathbf{x}_\alpha-\mathbf{v}_i t)]\}$$

and since the expansion of the rhs of this yields (2.3), we may write the contribution to the rhs of Eq. (2.2) in the simple form

$$C^{1-\mu} \int \prod_{i=1,\neq\alpha}^{\mu} d\mathbf{x}_i d\mathbf{v}_i X_{\eta\mu} \prod_{j=1,\neq\alpha}^{\mu} \delta(\mathbf{x}_\alpha-\mathbf{x}_j)$$

$$\times f_1(\mathbf{x}_j,\mathbf{v}_j,t) f_1(\mathbf{x}_\alpha,\mathbf{v}_\alpha,t), \quad (2.4)$$

where we have integrated over the velocities of the particles $\neq\alpha$, and have symmetrized the result by inserting the delta functions and integrating also over positions. It is to be noted that the factor $C^{1-\mu}$ is always canceled by a term $C^{\mu-1}$ in $X_{\eta\mu}$. But any term in (2.4) is proportional to C^μ through the C dependence of the f_1's.

Equations (2.2) and (2.4) thus give a formal representation of a "Boltzmann equation" to any order in either strength of interaction or concentration or both. In terms of operators it is easy to write, for example, the Boltzmann equation correct to order $C(Ct)^n$:

$$\frac{\partial f_1(\alpha)}{\partial t} + \mathbf{v}_\alpha\cdot\frac{\partial f_1(\alpha)}{\partial \mathbf{x}_\alpha}$$

$$= \int d\mathbf{x}_i d\mathbf{v}_i \Big(\bigcirc + \bigcirc\!\!\bigcirc + \bigcirc\!\!\bigcirc\!\!\bigcirc + \cdots \Big)$$

$$\times \delta(\mathbf{x}_\alpha-\mathbf{x}_i) f_1(i) f_1(\alpha) + \int d\mathbf{x}_i d\mathbf{v}_i d\mathbf{x}_j d\mathbf{v}_j$$

$$\times \Big(\circ + \ominus + \circ\!\!\circ + \ominus\!\!\circ + \cdots \Big) \delta(x_\alpha-\mathbf{x}_i)$$

$$\times \delta(\mathbf{x}_\alpha-\mathbf{x}_j) f_1(i) f_1(j) f_1(\alpha). \quad (2.5)$$

We have cancelled the powers of C in front of the integral with those in $X_{\eta\mu}$, in order to display more clearly the C dependence of the rhs of Eq. (2.5). Similar extensions to higher order are obvious.

3. DECAY OF INITIALLY PRESENT CORRELATIONS

We omit from consideration those diagrams of any order which have a vertex located off the skeleton, e.g.,

$\rho_{\mathbf{k}}(\alpha) =$  $\rho_{\mathbf{k}}(i),$

$\rho_{\mathbf{k}}(\alpha) =$  $\rho_{\mathbf{k}'}(\alpha)\rho_{(\mathbf{k}-\mathbf{k}')}(i).$

Such diagrams always introduce a factor of the order of $V_{\mathbf{k}} i\mathbf{k}\cdot\mathbf{D}_{\alpha i}$ times a slowly varying exponential. Even if such a contribution were multiplied by $\mathbf{v}t$, the result would still be much less than unity, because of the fundamental assumption on the size of $\mathbf{k}$.[2] This contribution could thus be thought of as giving an effective order t^{-1}, i.e., negligible for long times.

We now assert that initially present correlations in

an inhomogeneous system decay during exactly the same molecular relaxation time as was found for homogeneous systems,[4] i.e., we assert that the diagonal operator (cycle on a line) acting in the inhomogeneous case is just as effective in destroying correlations as it was in the homogeneous case. We give the proof for $f_2'(\alpha\beta)$ (in the notation of footnote reference 4), the proof for higher order correlations being then obvious.

With the cycle on the line there is the possibility of particle i having wave vector initially either zero or of macroscopic size (pseudodiagonal) (see Diagram 1).

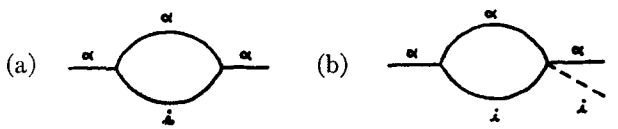
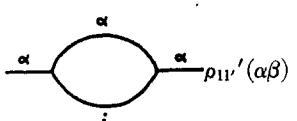


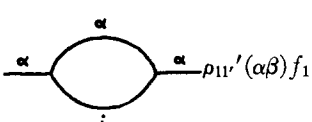
DIAGRAM 1. Possible cycle on line diagrams which destroy initial correlations in inhomogeneous systems. The dashed line represents a "pseudodiagonal" propagation line. See Eq. (3.1).

The sole question is whether both diagrams in Diagram 1 destroy the initial correlation as quickly as Diagram 1(a) alone does in the homogeneous case.[4] Our proof follows closely that of footnote reference 4. Considering this combination, we are lead to the evolution equation (a similar operator involving particle β of course could be treated):

$$\frac{\partial\rho_{11'}'(\alpha\beta)}{\partial t}=$$



$$\times\{\rho_0(i)+\Omega^{-1}\sum_{\mathbf{k}}\rho_{\mathbf{k}}(i)\exp[i\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{v}_i t)]\}$$



$$=\rho_{11'}'(\alpha\beta)f_1(i)C^{-1}, \tag{3.1}$$

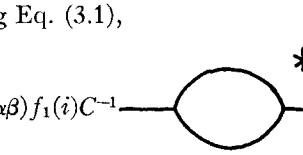
where the final replacement is made using Eq. (2.1).

We know that $f_1(i)$ changes only slowly with time $=0(t_h)\gg t_r$ in which we are interested. Thus $f_1(i)$ may be considered constant in this proof. We define the function

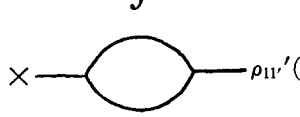
$$\Theta=\int d\mathbf{v}\rho_{11'}'(\alpha\beta)f_1(i)C^{-1}\rho_{11'}'(\alpha\beta)^*. \tag{3.2}$$

Therefore, using Eq. (3.1),

$$\frac{\partial\Theta}{\partial t}=\int d\mathbf{v}\rho_{11'}'(\alpha\beta)f_1(i)C^{-1}$$



$$\times\rho_{11'}'(\alpha\beta)^*f_1(i)^*C^{-1}+\int d\mathbf{v}\rho_{11'}'(\alpha\beta)^*f_1(i)^*C^{-1}$$



$$\times\rho_{11'}'(\alpha\beta)f_1(i)C^{-1},$$

where we made use of the reality of $f_1(i)$. Using the expression of the operator,[1,3,4] this becomes

$$\frac{\partial\Theta}{\partial t}\cong-2\int d\mathbf{v}d\mathbf{l}''|V_{1''}|^2\delta(\mathbf{l}''\cdot\mathbf{g}_{\alpha i})$$
$$\times|\mathbf{l}''\cdot\mathbf{D}_{\alpha i}\exp(-i\mathbf{l}\cdot\mathbf{v}_\alpha t)\rho_{11'}'(\alpha\beta)f_1(i)C^{-1}|^2.$$

By definition of relaxation time as the time during which initially present molecular correlations are adjusted,

$$\partial\Theta/\partial t=0,\quad t>t_r.$$

Therefore

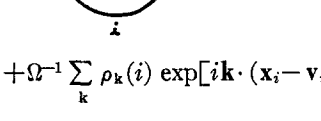
$$\exp(-i\mathbf{l}\cdot\mathbf{v}_\alpha t)\rho_{11'}'(\alpha\beta)f_1(i)C^{-1}=\Phi(H_0)A(t,\mathbf{x});\qquad t>t_r \tag{3.3}$$

where H_0 is the unperturbed Hamiltonian, i.e., all velocity dependence of the lhs of Eq. (3.3) rests in a function of $\sum_i v_i^2$. Differentiating Eq. (3.3) with respect to time, $-i\mathbf{l}\cdot\mathbf{v}_\alpha\Phi(H_0)A(t,\mathbf{x})$

$$+\exp(-i\mathbf{l}\cdot\mathbf{v}_\alpha t)\frac{\partial}{\partial t}\rho_{11'}'(\alpha\beta)f_1(i)C^{-1}$$
$$=\Phi(H_0)\frac{\partial}{\partial t}A(t,\mathbf{x}). \tag{3.4}$$

The second term of Eq. (3.4) can be shown to be zero:

$$\frac{\partial}{\partial t}\rho_{11'}'(\alpha\beta)f_1(i)C^{-1}$$



$$=f_1(i)C^{-2}\int d\mathbf{l}''|V_{1''}|^2\exp(i\mathbf{l}\cdot\mathbf{v}_\alpha t)\mathbf{l}''\cdot\mathbf{D}_{\alpha i}$$
$$\times\delta(\mathbf{l}''\cdot\mathbf{g}_{\alpha i})\mathbf{l}''\cdot\mathbf{D}_{\alpha i}\exp(-i\mathbf{l}\cdot\mathbf{v}_\alpha t)\rho_{11'}'(\alpha\beta)f_1(i)$$
$$=f_1(i)C^{-2}\int d\mathbf{l}''|V_{1''}|^2\exp(i\mathbf{l}\cdot\mathbf{v}_\alpha t)\mathbf{l}''\cdot\mathbf{D}_{\alpha i}$$
$$\times\delta(\mathbf{l}''\cdot\mathbf{g}_{\alpha i})\mathbf{l}''\cdot\mathbf{D}_{\alpha i}\Phi(H_0)A(t,\mathbf{x})$$
$$=f_1(i)C^{-2}\int d\mathbf{l}''|V_{1''}|^2\exp(i\mathbf{l}\cdot\mathbf{v}_\alpha t)\mathbf{l}''\cdot\mathbf{D}_{\alpha i}$$
$$\times\delta(\mathbf{l}''\cdot\mathbf{g}_{\alpha i})\mathbf{l}''\cdot\mathbf{g}_{\alpha i}\Psi(\mathbf{v},\mathbf{x},t)=0.$$

Equation (3.4) thus becomes

$$\begin{aligned}&\partial A(\mathbf{x},t)/\partial t=-i\mathbf{l}\cdot\mathbf{v}_\alpha A(\mathbf{x},t),\quad t>t_r\\&A(t)/A(t_r)=\exp[-i\mathbf{l}\cdot\mathbf{v}_\alpha(t-t_r)].\end{aligned} \tag{3.5}$$

Equation (3.3) says that at *no* time $t>t_r$ may A be a function of velocity. Yet Eq. (3.5) gives velocity dependence, since the molecular wave vectors are such that $\mathbf{l}\cdot\mathbf{v}t_r\gg1$.[2] Putting $A=0$ in Eq. (3.3) gives

$$\rho_{11'}'(\alpha\beta)=0,\quad t>t_r. \tag{3.6}$$

Thus initially present correlations are destroyed in an inhomogeneous system by the same scattering mechanism and during the same relaxation time as correlations in homogeneous systems. Only creation fragments[4] can contribute to correlations after such a time.

4. CORRELATIONS ARISING IN INHOMOGENEOUS SYSTEMS

We define a reduced s-particle distribution function by

$$f_s(\mathbf{x}_1,\mathbf{v}_1,\cdots\mathbf{x}_s,\mathbf{v}_s,t)$$

$$=C^s\Big\{\prod_{i=1}^{s}\rho_0(i)+\sum_{i=1}^{s}\prod_{j=1,\neq i}^{s}\rho_0(j)\Omega^{-1}\sum_{\mathbf{n}}\rho_{\mathbf{n}}(i)$$

$$\times\exp[i\mathbf{n}\cdot(\mathbf{x}_i-\mathbf{v}_it)]+\sum_{i<j=1}^{s}\prod_{m=1,\neq i,j}^{s}\rho_0(m)\Omega^{-2}$$

$$\times\sum_{\mathbf{n},\mathbf{n}'}\rho_{\mathbf{n}\mathbf{n}'}(ij)\exp[i\mathbf{n}\cdot(\mathbf{x}_i-\mathbf{v}_it)+i\mathbf{n}'\cdot(\mathbf{x}_j-\mathbf{v}_jt)]$$

$$+\sum_{i<j=1}^{s}\prod_{m=1,\neq i,j}^{s}\rho_0(m)\Omega^{-1}\sum_{\mathbf{n}}\rho_{\mathbf{n},-\mathbf{n}}(ij)$$

$$\times\exp[i\mathbf{n}\cdot(\mathbf{x}_i-\mathbf{v}_it)-i\mathbf{n}\cdot(\mathbf{x}_j-\mathbf{v}_jt)]+\cdots$$

$$+\Omega^{-s}\sum_{\{\mathbf{n}_s\}}\rho_{\{\mathbf{n}_s\}}(\{s\})\exp[i\sum_{i=1}^{s}\mathbf{n}_i\cdot(\mathbf{x}_i-\mathbf{v}_it)]\Big\}. \quad (4.1)$$

We shall prove that for times t such that $t_h>t>t_r$, Eq. (4.1) may be expressed as a complicated, *but completely determined*, functional of a product of singlet distribution functions. Thus all the time dependence of (4.1) will rest in the individual $f_1(i)$.

The terms in Eq. (4.1) which contain only $\rho_{\mathbf{k}}$'s and ρ_0's factorize.[2] The terms left over have at least two molecularly correlated particles. For those with just two, the nonmolecularly correlated part again factorizes. Similarly for those with just three, etc. We can write

$$f_s=\prod_{i=1}^{s}f_1(i)+C^2\sum_{i<j=1}^{s}G_2(ij)]\prod_{n=1,\neq i,j}^{s}f_1(n)$$

$$+C^3\sum_{i<j<m=1}^{s}G_3(ijm)\prod_{n=1,\neq i,j,m}^{s}f_1(n)+\cdots+C^sG_s, \quad (4.2)$$

where $G_j(\{j\})$ represents the sum of terms in the $\{\ \}$ of Eq. (4.1) in which $\mathbf{l}$ vectors occur for the set of particles $\{j\}$ and either $\mathbf{k}$ vectors or zero wave vector for the rest of the s particles.

We shall prove G_u a functional of a product of f_1's. G_u can be formed only by a creation operator creating u correlated particles[4] acting on

$$\prod_{m=1}^{v}\rho_0(m)+\sum_{i=1}^{v}\prod_{m=1}^{v}\rho_0(m)\exp(-i\mathbf{k}_i\cdot\mathbf{v}_it)\rho_{\mathbf{k}_i}(i)$$

$$+\sum_{i<j=1}^{v}\prod_{m=1,\neq i,j}^{v}\rho_0(m)\exp[-i(\mathbf{k}_i\cdot\mathbf{v}_i+\mathbf{k}_j\cdot\mathbf{v}_j)t]$$

$$\times\rho_{\mathbf{k}_i}(i)\rho_{\mathbf{k}_j}(j)+\cdots+\sum_{i=1}^{v}[\rho_{\mathbf{k}_i}(i)\exp(-i\mathbf{k}_i\cdot\mathbf{v}_it)], \quad (4.3)$$

where v particles are involved in the creation operator ($v\geq u$). Consider separately the operator acting on each term in (4.3). In each term the sum of the $\mathbf{l}$ vectors of the correlation [the exponentials of Eq. (4.1), which are to the left of the operator] equals the sum of the $\mathbf{k}$ vectors of the term in (4.3). From the exponentials in $\mathbf{l}$ on the left we factor a term $\exp(i\mathbf{k}_i\cdot\mathbf{x}_i)$ for each exponential to the right of the operator and commute it with the operator. For particles in $\{v\}$ not in $\{u\}$, we are free to choose any one of the particles on the left. We do this arbitrarily, selecting particle α. After this, the $\mathbf{l}$ vectors on the left always sum to zero, and each exponential on the right is either

$$\exp[i\mathbf{k}_i\cdot(\mathbf{x}_i-\mathbf{v}_it)] \quad \text{or} \quad \exp[i\mathbf{k}_i\cdot(\mathbf{x}_\alpha-\mathbf{v}_it)],$$

depending as i is or is not contained in $\{u\}$. We give this alternative the notation $\exp[i\mathbf{k}_i\cdot(\mathbf{x}_i^*-\mathbf{v}_it)]$.

The operator which takes the set of wave numbers $\{\mathbf{k}_i\}$ into the set $\mathbf{l}_u$ is[1,3]

$$\Omega^{-i}\sum_{\mathbf{k}_i}\langle\{l_u\}\,|\,\mathrm{X}_{\eta\mu}'\,|\,\{\mathbf{k}_i\}\rangle\delta^{kr}(\sum_u\mathbf{l}_u-\sum_i\mathbf{k}_i).$$

Because of the smallness of the $\mathbf{k}$ vectors, the matrix element as written is essentially independent of the $\{\mathbf{k}_i\}$. We call this operator $\mathrm{X}_{\eta\mu}'$. Also, so far as the sum over $\{\mathbf{l}_u\}$ demanded by Eq. (4.1) is concerned,

$$\delta^{kr}(\sum_u\mathbf{l}_u-\sum_i\mathbf{k}_i)\cong\delta^{kr}(\sum_{\{u\}}\mathbf{l}_u)$$

and this δ^{kr} commutes with the operator. This imposes a limitation on the summation over $\mathbf{l}$ vectors which was not intended in the original Eq. (4.1). The only way to abide strictly by (4.1) is to sum over the $\mathbf{l}$ vectors with the δ^{kr} and also to sum over all the $\mathbf{k}$ vectors for each excited particle on the right. We now write

$$G_u=\Omega^{-u}\sum_{\{\mathbf{l}_u\}}\exp(i\sum_{\{u\}}\mathbf{l}_u\cdot\mathbf{x}_u)\delta^{kr}(\sum_{\{u\}}\mathbf{l}_u)\mathrm{X}_{\eta\mu}'$$

$$\times\Big\{\prod_{m=1}^{v}\rho_0(m)+\sum_{i=1}^{v}\prod_{m=1,\neq i}^{v}\rho_0(m)\Omega^{-1}$$

$$\times\sum_{\mathbf{k}_i}\exp[i\mathbf{k}_i\cdot(\mathbf{x}_i-\mathbf{v}_it)]\rho_{\mathbf{k}_i}(i)$$

$$+\sum_{i<j=1}^{v}\prod_{m=1,\neq i,j}^{v}\rho_0(m)\Omega^{-2}$$

$$\times\sum_{\mathbf{k}_i,\mathbf{k}_j}\exp[i\mathbf{k}_i\cdot(\mathbf{x}_i-\mathbf{v}_it)+i\mathbf{k}_j\cdot(\mathbf{x}_j-\mathbf{v}_jt)]$$

$$+\cdots+\prod_{i=1}^{v}\{\Omega^{-1}\sum_{\mathbf{k}_i}\exp[i\mathbf{k}_i\cdot(\mathbf{x}_i^*-\mathbf{v}_it)]\}. \quad (4.4)$$

If we integrate (4.4) over $\mathbf{x}_j$ (all j not included in $\{u\}$) inserting $\delta(\mathbf{x}_\alpha-\mathbf{x}_j)$ in the integrand, and change $\mathbf{x}_\alpha$ where it appears to $\mathbf{x}_j$, Eq. (4.4) can be simply written, using Eq. (2.1),

$$G_u=C^{-v}\Omega^{-u}\int\prod_{\substack{m=1\\ \neq\{u\}}}^{v} d\mathbf{v}_m\sum_{\{l_u\}}\exp(i\sum_{\{u\}}\mathbf{l}_u\cdot\mathbf{x}_u)\delta^{kr}(\sum_{\{u\}}\mathbf{l}_u)\mathrm{X}_{\eta\mu}' \times\int\prod_j d\mathbf{x}_j\delta(\mathbf{x}_\alpha-\mathbf{x}_j)\prod_{i=1}^{v} f_1(i). \quad (4.5)$$

We have thus shown G_u to be a time-independent functional of the product of a number of f_1's, this number being determined by the order in concentration of the approximation to which we are calculating. Coupling (4.5) with Eq. (4.2) gives the entire f_s as a similar functional.

To illustrate, we write the equation similar to (2.5) for the doublet distribution function f_2

$$f_2(\alpha\beta)=f_1(\alpha)f_1(\beta)+\int d\mathbf{k}e^{-i\mathbf{k}\cdot\mathbf{R}}\left(>+\bigcirc\!\!>+\bigcirc\!\!\bigcirc\!\!>+\cdots\right)f_1(\alpha)f_1(\beta)$$

$$+\int d\mathbf{k}d\mathbf{v}_i e^{-i\mathbf{k}\cdot\mathbf{R}}\left(>+\bigcirc\!\!>+\bigtriangleup\!\!>+\cdots\right)\int d\mathbf{x}_i\delta(\mathbf{x}_i-x_\alpha)f_1(i)f_1(\alpha)f_1(\beta)+\cdots. \quad (4.6)$$

The physical meaning of the operators of the rhs has been studied.[3,7]

5. DISCUSSION

We have seen that during an initial period $t<t_r$, an arbitrarily given hydrodynamic system evolves in a manner characterized by the destruction of initially present correlations and the formation of those correlations characteristic of local equilibrium. During this period, normal thermodynamic functions such as entropy would be difficult to define. For $t>t_r$, the complete time dependence of any reduced distribution function rests in a product of singlet distribution functions. These singlet functions evolve solely through dependence on themselves and other singlet functions. We have thus found the specific form of the functional relationships suggested by Bogoliubov.[6]

[7] F. C. Andrews, Acad. roy. Belg. Classe sci. (to be published).

The formal equations in terms of Prigogine diagrams, which can now be written down to any desired order in either strength of coupling or concentration, represent a starting point for a review of all of transport theory. We are ready to start summing diagrams and considering various potential models in studying the various transport processes to place them on a sound basis, i.e., derived directly from the Liouville equation the mechanical equation of motion.

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Molecular Collisions. II. Diatomic Molecules*†

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A set of coupled integral equations describing the collisions of diatomic molecules is developed by exploitation of the properties of the irreducible representations of the three-dimensional rotation group. An expansion of the cross section in spherical harmonics is described, and its virtues argued.

THE first paper[1] of this series presented a formal theory of inelastic molecular collisions. In this paper we develop the theory further for the case of diatomic molecules.

The basis of this development, as in several earlier papers,[2–4] lies in the exploitation of the properties of the irreducible representations of the three-dimensional rotation group. In these early papers the wave equation was interpreted as a differential equation, so that the representation coefficients needed to be differentiated. In the present paper we use an integral equation formulation, and are thus left with the much simpler problem of integrating the representation coefficients. Both methods lead to sets of coupled equations, differential equations in the one case and integral equations in the other, and we have shown that the two methods are equivalent.[5] Though no new results are derived in this paper from the integral equation approach, it is presented as an example of a powerful mathematical technique, which is susceptible to generalization.

The remaining part of the paper relates the cross sections to the asymptotic forms of the solutions of the equations mentioned previously. An expansion of the cross sections in the representation coefficients leads to a set of cross section coefficients expressible to a large extent in terms of group theoretical variables, and thus dependent in a simple way on the chemical nature of the molecules involved. The expansion has the further virtue that the averaged cross sections of interest in the kinetic theory involve only the first few coefficients, and are exactly expressible in terms of these coefficients.

1. INTRODUCTION

We wish to study the collisions of two diatomic molecules. The results must be of the form of cross sections for the occurrence of certain final states, given the initial state. The specification of the initial state includes the rotational and vibrational states of each molecule, the kinetic energy, and the direction of motion of one molecule relative to the other. This last is not arbitrary, since an objective direction in space is provided by the quantization of the rotational states.

What is desired is the cross section per unit solid angle for scattering in a given direction, with the molecules in given rotational and vibrational states. The kinetic energy is known from knowledge of the internal energies and the fact that the total energy must be conserved.

Quite often only the energy of an internal state is of interest, because the degenerate states are equally probable. In that case the proper cross section is one averaged over initial states and summed over final. The reason for the lack of symmetry between initial and final lies in that for any cross sections we count the *total* number of final states for *unit* initial flux. This question is considered in some detail later.

We will rely on the terminology and concepts of the three-dimensional rotation group. One point which must be stressed is the distinction between point transformations and coordinate transformations. In what follows we use point transformations, for various reasons, the most important of which is that the internal energy states must be quantized relative to fixed axes. Thus our rotations are rotations of the whole space, carrying material bodies with them, and the coordinate system remains fixed.

Our conventions and terminology are those of the English edition of Wigner's book on group theory.[6]

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* In part, this paper is based on a thesis [University of Wisconsin, Naval Research Laboratory Rept. WIS-NSF-5 (1955)] submitted by George Gioumousis to the University of Wisconsin in partial fulfillment of the requirements of a Ph.D. degree in theoretical chemistry.

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[1] G. Gioumousis and C. F. Curtiss, J. Chem. Phys. **29**, 996 (1958). This paper will be referred to as I, and equations from it as I-(35), etc.

[2] C. F. Curtiss, J. O. Hirschfelder, and F. T. Adler, J. Chem. Phys. **18**, 1638 (1950).

[3] C. F. Curtiss and F. T. Adler, J. Chem. Phys. **20**, 249 (1952).

[4] C. F. Curtiss, J. Chem. Phys. **21**, 2045 (1953).

[5] G. Gioumousis, University of Wisconsin Naval Research Laboratory Rept. WIS-NSF-5 (1955).

[6] E. Wigner, *Group Theory* (Academic Press, Inc., New York, 1959).

Other references are Rose,[7] Edmonds,[8] and Hirschfelder *et al.*[9] A rotation is parametrized in terms of Eulerian angles, which are defined by the following factorization of the rotation matrix R:

$$R=R(\alpha\beta\gamma)=\begin{bmatrix}\cos\alpha & \sin\alpha & 0\\ -\sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}\cos\beta & 0 & -\sin\beta\\ 0 & 1 & 0\\ \sin\beta & 0 & \cos\beta\end{bmatrix}\begin{bmatrix}\cos\gamma & \sin\gamma & 0\\ -\sin\gamma & \cos\gamma & 0\\ 0 & 0 & 1\end{bmatrix}, \tag{1.1}$$

where $0\leq\alpha\leq 2\pi$, $0\leq\beta\leq\pi$, and $0\leq\gamma\leq 2\pi$. The inverse matrix R^{-1} is given by

$$R(\alpha\beta\gamma)^{-1}=R(2\pi-\gamma\pm\pi,\ \beta,\ 2\pi-\alpha\pm\pi), \tag{1.2}$$

where the plus or minus sign is chosen as needed to keep the argument in the proper range. It is worthy of note that the rotation $R(\alpha\beta\gamma)$ which rotates a vector $\mathbf{v}$ to coincidence with the upper half of the z axis has Eulerian angles β, γ which are equal to the polar angles θ, φ of the vector. Thus, when convenient, directions in space will be given in terms of rotations.

A critical point is that the Hamiltonian of the system of two colliding particles is invariant to the rotations of the whole system.[10] This follows from the fact that it is an isolated system. As a result the representations of the rotation group (since they do form a complete, orthogonal set over the group) are the natural set for series expansions. Following Wigner[6] we denote the elements of the $2j+1$-dimensional matrix representation by

$$D^j(R)_{nm} \quad \text{or} \quad D(jnm|R),$$

where the latter form is preferred for complex expressions. We use only the simplest properties of the matrix representations, e.g., the orthogonality with respect to integration over the group and the matrix relation

$$D^j(RS)=D^j(R)D^j(S).$$

The Clebsch-Gordan series is written in the form

$$D^{j_1}(R)_{n_1m_1}D^{j_2}(R)_{n_2m_2}=\Sigma_J\, C(j_1j_2J;\, n_1+n_2,\, m_1+m_2)\times D^J(R)_{n_1+n_2,m_1+m_2}.$$

We use Rose's[7] $C(jj'J;nn')$ rather than Wigner's[6] $s_{Jnn'}{}^{ii'}$ for typographical convenience.[11]

With the foregoing nomenclature settled, it is possible to set up a flexible and powerful set of coordinates for the problem at hand, which is the interaction of a pair of diatomic molecules. Let the molecules be labeled a and b, with atoms a_1, a_2 and b_1, b_2, respectively. Let the vector from the center of mass of a to the center of mass of b be $\mathbf{r}$, the vector from a_1 to a_2 be $\mathbf{r}^a$ and the vector from b_1 to b_2 be $\mathbf{r}^b$. Let the polar forms of these vectors be $(r\theta\varphi)$, $(r^a\theta^a\varphi^a)$, and $(r^b\theta^b\varphi^b)$. Further, let the rotations R, R^a, R^b be defined such as to place the respective vectors parallel to the positively directed z axis. This defines the rotations except for the first Eulerian angle, that written as α previously. For R, this angle is defined by the requirement that the rotation put the vector $\mathbf{r}^a$ in the left half ($x<0$, $y=0$) of the xz plane. The first Eulerian angles for the rotations R^a, R^b are taken to be zero.

It is also convenient to use a pair of rotations to specify the orientation of the two molecules $\mathbf{r}^a$, $\mathbf{r}^b$ relative to the intermolecular axis. First let the rotation R be performed on the whole system, then let S^a, S^b be the rotations that bring $\mathbf{r}^a$, $\mathbf{r}^b$ parallel to the z axis. Just as with R^a, R^b, the first Eulerian angles are arbitrary and are put equal to zero. From the definition of the first Eulerian angle of R, it is seen that the third Eulerian angle of S^a is zero. The second Eulerian angle of $S^a(S^b)$ is the angle between $\mathbf{r}$ and $\mathbf{r}^a(r^b)$, while the third angle of S^b is the azimuthal angle between $\mathbf{r}^a$ and $\mathbf{r}^b$. It is evident that

$$R^a=S^aR, \quad \text{and} \quad R^b=S^bR.$$

Similarly, rotations can be used to describe the direction of motion of the molecules before and after the collision. The desired cross sections will have the form

$$\sigma(n^al^am^a;\, n^bl^bm^b;\, T|\,E\,|n^{a\prime}l^{a\prime}m^{a\prime};\, n^{b\prime}l^{b\prime}m^{b\prime};\, T').$$

Here nlm are the usual quantum numbers of a vibrating rotating molecule. The rotation T is such as to make the velocity of b relative to that of a parallel to the z axis, and E is the total energy of the collision. Primed variables refer to the values after the collision.

2. EXPANSIONS IN THE $D(lmn/R)$

The internal wave functions have the form[12]

$$Y(lm|R^a)Z(nl|r^a)=(2l+1)^{\frac{1}{2}}(4\pi)^{-\frac{1}{2}}\times D(l0m|R^a)Z(nl|r^a), \tag{2.1}$$

where the Y is the usual spherical harmonic of the second two Eulerian angles of R^a, and $Z(nl|r^a)$ is the oscillator wave function. These functions will appear as a product of a pair of internal wave functions with a plane wave function. We have for the latter[13]

$$e^{i\mathbf{k}\cdot\mathbf{r}}=\Sigma_L(2L+1)J(L|kr)P_L(\cos\Theta),$$

[7] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

[8] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

[9] J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *The Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954).

[10] Let it be emphasized that this is a physical statement, not one about coordinate transformations. Any Hamiltonian is invariant to coordinate transformations, as is well known.

[11] See also E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, New York, 1935).

[12] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949).

[13] G. M. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, New York, 1952).

where Θ is the angle between $\mathbf{k}$ and $\mathbf{r}$, $j(L|\cdots)$ the spherical Bessel function[12] and P_L the Legendre polynomial. If T is the rotation which puts $\mathbf{k}$ parallel to the z axis, then Θ is the middle Eulerian angle of RT^{-1}, thus

$$P_L(\cos\Theta)=D(L00|RT^{-1})$$
$$=\sum_s(-1)^s D(L0s|R)D(L0-s|T),$$

which yields the following expansion for a plane wave function,

$$e^{i\mathbf{k}\cdot\mathbf{r}}=\sum_{Ls} i^L(-1)^s(2L+1)D(L0s|R)$$
$$\times D(L0-s|T)j_L(kr). \quad (2.2)$$

The Green's function to be used later may be expanded similarly. The following is a well-known series written in a somewhat unusual form,[13,14]

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}=ik\sum_l(2l+1)j_l(kr_<)h_l(kr_>)P_l(\cos\Phi),$$

where Φ is the angle between the vectors $\mathbf{r}$ and $\mathbf{r}'$, $r_<$ the lesser of r and r', and $r_>$ the greater. The Legendre polynomial may be written in terms of the rotations R and R' just as previously with result

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}=ik\sum_{ls}(2l+1)j_l(kr_<)h_l(kr_>)(-1)^s$$
$$\times D(l0s|R)D(l0-s|R'). \quad (2.3)$$

The intermolecular potential energy function, which in I was simply denoted by V, here is a function of r, r^a, r^b, S^a, S^b only. The dependence of $V(rr^ar^bS^aS^b)$ on the rotations can be expressed in terms of an expansion in the irreducible representations. Of the many possible forms the following seems to be the most convenient:

$$V(rr^ar^bS^aS^b)=\sum_{l_1l_2\mu_2} v(l_1l_2\mu_2|rr^ar^b)$$
$$\times D(l_10-\mu_2|S^a)D(l_20\mu_2|S^b); \quad (2.4)$$

however, at several points in what follows it will be necessary that all functions be expressed in terms of R, R^a, R^b, which may be done by use of the equation $S^a=R^aR^{-1}$, the corresponding equation for S^b, and the defining property of a matrix representation, that group multiplication corresponds to matrix multiplication. The result is

$$V(rr^ar^bS^aS^b)=\sum_{l_1l_2\mu_2s_1s_2}(-1)^{s_1+s_2}v(l_1l_2\mu_2|rr^ar^b)$$
$$\times D(l_10s_1|R^a)D(l_20s_2|R^b)$$
$$\times D(l_1\mu_2-s_1/R)D(l_1-\mu_2-s_2|R). \quad (2.5)$$

At this point there are three rotating systems to be considered: the two molecules and the rotation of one molecule relative to the other. It will be found to be convenient to couple these three systems into a state with sharp total angular momentum. By the rule for composition of angular momenta, the function

$$I(l^al^bl\lambda LM|RR^aR^b)$$
$$=\sum_{m^am} C(l\lambda Lm, M-m)C(l^al^blm^a, m-m^a)$$
$$\times D(l^a0m^a|R^a)D(l^bD, m-m^a|R^b)$$
$$\times D(\lambda0, M-m|R) \quad (2.6)$$

represents a state where a and b have been coupled to give a state with total angular momentum l, and z component m and this state in turn is coupled with the relative rotation to give total angular momentum L, and z component M. The equation may be inverted to give

$$D(l^a0m^a|R^a)D(l^b0m^b|R^b)D(\lambda0\mu|R)$$
$$=\sum_{lL} C(l\lambda L, m^a+m^b, \mu)C(l^al^blm^am^b)$$
$$\times I(l^al^bl\lambda L, m^a+m^b+\mu|RR^aR^b). \quad (2.7)$$

As before, it is well to express the function I in terms of RS^aS^b instead of RR^aR^b, with result

$$J(l^al^bl\lambda LM|RS^aS^b)$$
$$=I(l^al^bl\lambda LM|R,S^aR,S^bR)$$
$$=\sum_{m^amst} C(l\lambda Lm, M-m)C(l^al^blm^am-m^a)$$
$$\times D(l^a0s|S^a)D(l^b0t|S^b)D(l^asm^a|R)$$
$$\times D(l^bt, m-m^a|R)D(\lambda0, M-m|R).$$

The Clebsch-Gordan series may be applied twice in succession to the product of representation coefficients involving R, so that (dropping the RS^aS^b dependence for the time being)

$$J(l^al^bl\lambda LM)=\sum_{\substack{m^ams\\ ll_3l_4}} C(l\lambda Lm, M-m)C(l^al^blm^a, m-m^a)$$
$$\times D(l^a0s|S^a)D(l^b0t|S^b)C(l^al^bl_3st)$$
$$\times C(l^al^bl_3m^a, m-m^a)C(l_3\lambda l_4, s+t, 0)$$
$$\times C(l_3\lambda l_4m, M-m)D(l_4, s+t, M|R).$$

By the orthogonality rules[6] for the Clebsch-Gordan coefficients, the sums in m^a and m become δll_3 and δl_4L, respectively, giving the following expression for J

$$J(l^al^bl\lambda LM|RS^aS^b)$$
$$=\sum_{st} C(l^al^blst)C(l\lambda L, s+t, 0)D(l^a0s|S^a)$$
$$\times D(l^b0t|S^b)D(L, s+t, M|R), \quad (2.8)$$

which is the simplest expression of the form desired.

[14] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953).

3. THE INTEGRAL EQUATIONS

In I, the integral equation

$$\psi_i=\varphi_i+G^+V\psi_i \tag{3.1}$$

was set up to be solved with the initial state φ_i a plane wave, that is, with sharp linear momentum. Here the resulting equations are simpler if the integral equation is taken with φ_i of sharp angular momentum, and the wave functions originally desired then built up by linearity. The initial state then will have the form

$$\begin{aligned}\varphi_i&=\varphi(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M}\,|\,RR^aR^brr^ar^b)\\&=Z(\bar{n}^a\bar{l}^a\,|\,r^a)Z(\bar{n}^b\bar{l}^b\,|\,r^b)j(\bar{L}\,|\,kr)I(\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M}\,|\,RR^aR^b).\end{aligned} \tag{3.2}$$

The use of Eq. (2.2) to form a plane wave from a linear combination of these functions will be discussed in Sec. 4.

It is better here to work with the operator $G^+(E)$ directly, which can be done if it is written as the usual bilinear series for the part which is a function of internal variables. Thus

$$\begin{aligned}&G^+(E)f(\mathbf{r}r^ar^bR^aR^b)\\&=\left(\frac{1}{2\pi}\right)^2\int\int\int\sum_{\substack{n^al^am^a\\n^bl^bm^b}}Y(l^am^a\,|\,R^a)Y(l^am^a\,|\,R^{a'})^*\\&\times Y(l^bm^b\,|\,R^b)Y(l^bm^b\,|\,R^{b'})^*Z(n^al^a\,|\,r^a)Z(n^al^a\,|\,r^{a'})^*\\&\times Z(n^bl^b\,|\,r^b)Z(n^bl^b\,|\,r^{b'})^*\left(-\frac{\mu}{2\pi\hbar^2}\cdot\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\right)\\&\times f(\mathbf{r}'r^ar^{b'}R^{a'}R^{b'})d\mathbf{r}dr^{a'}dr^{b'}dR^{a'}dR^{b'}.\end{aligned}$$

Here the wave number is defined in the obvious manner,[1] as in Eq. I-(2.2), that is,

$$\tfrac{1}{2}\mu k^2=\tfrac{1}{2}\mu k(n^al^an^bl^b)^2=E-E^a-E^b.$$

The factor $(1/2\pi)^2$ occurs because the spherical harmonics are normalized to unity when integrated over two Eulerian angles, while the present integration is over three.

The operator may be put in better form by use of Eqs. (2.1) and (2.3). In addition, the dummy indices $n^al^am^an^bl^bm^b$ are changed to $n_1l_1m_1n_2l_2m_2$. Thus

$$\begin{aligned}G^+(E)f=&\frac{1}{2\pi}\int\cdots\int\sum_{\substack{ll_2n_1n_2\\m_1m_2ls}}ik\left(\frac{-\mu}{2\pi\hbar^2}\right)\\&\times\frac{(2l_1+1)(2l_2+1)(2l+1)}{(8\pi^2)^2}Z(n_1l_1\,|\,r^a)\\&\times Z(n_2l_2\,|\,r^b)D(l0s\,|\,R)D(l_10m_1\,|\,R^a)\\&\times D(l_20m_2\,|\,R^b)Z(n_1l_1\,|\,r^{a'})^*Z(n_2l_2\,|\,r^{b'})^*\\&\times D(l0s\,|\,R')^*D(l_10m_1\,|\,R^{a'})^*D(l_20m_2\,|\,R^{b'})^*\\&\times j_l(kr_<)h_l(kr_>)f(\mathbf{r}'r^{a'}r^{b'}R^{a'}R^{b'})\\&\times r'^2dr'dR'dr^{a'}dr^{b'}dR^{a'}dR^{b'},\end{aligned}$$

where the energy dependence of $G^+(E)$ is evidenced only through $k=k(n_1l_1n_2l_2)$. By use of Eq. (2.1) twice, and the orthogonality of the Clebsch-Gordan coefficients, the operator becomes

$$\begin{aligned}G^+(E)f=&\frac{1}{2\pi}\int\cdots\int\sum_{\substack{l_1l_2l_3l_4\\l_5Mn_1n_2}}\left(-\frac{\mu ki}{2\pi\hbar^2}\right)\\&\times\frac{(2l_1+1)(2l_2+1)(2l_5+1)}{(8\pi^2)^2}j_{l_5}(kr_<)h_{l_5}(kr_>)\\&\times I(l_1l_2l_3l_5l_4M\,|\,RR^aR^b)I(l_1l_2l_3l_5l_5M\,|\,R'R^{a'}R^{b'})^*\\&\times Z(n_1l_1\,|\,r^a)Z(n_1l_1\,|\,r^{a'})^*Z(n_2l_2\,|\,r^b)\\&\times Z(n_2l_2\,|\,r^{b'})^*f(r'r^{a'}r^{b'}R'R^{a'}R^{b'})\\&\times r'^2dr'dr^{a'}dr^{b'}dR'dR^{a'}dR^{b'}.\end{aligned} \tag{3.3}$$

By a basic property of group integration, the integral can be expressed in terms of $R'S^{a'}S^{b'}$, with

$$dR'dS^{a'}dS^{b'}=dR'dR^{a'}dR^{b'}. \tag{3.4}$$

Then, if the functions $I(\cdots\,|\,RR^aR^b)$ are replaced by $J(\cdots\,|\,DS^aS^b)$, the entire operator can be expressed in terms of RS^aS^b instead of RR^aR^b, a change of variable which turns out to be quite convenient.

The wave function is expanded in terms of the I's as

$$\begin{aligned}\psi=&\sum_{\substack{n^{a''}n^{b''}l^{a''}l^{b''}l''\\\lambda''L''M''}}\psi(n^{a''}n^{b''}l^{a''}l^{b''}l''\lambda''L''M''\,|\,r)Z(n^{a''}l^{a''}\,|\,r^a)\\&\times Z(n^{b''}l^{b''}\,|\,r^b)I(l^{a''}l^{b''}l''\lambda''L''M''\,|\,RR^aR^b).\end{aligned} \tag{3.5}$$

Substitution of Eqs. (3.5), (3.2), (3.3), and (2.4) in Eq. (3.1) yields the integral equation in series form, after due notice is taken of Eqs. (2.7) and (3.4).

$$\begin{aligned}&\sum_{\substack{n^{a''}n^{b''}l^{a''}l^{b''}\\l''\lambda''L''M''}}\psi(n^{a''}n^{b''}l^{a''}l^{b''}l''\lambda''M''\,|\,r)Z(n^{a''}l^{a''}\,|\,r^a)\\&\times Z(n^{b''}l^{b''}\,|\,r^b)I(l^{a''}l^{b''}l''\lambda''L''M''\,|\,RR^aR^b)\\&=Z(\bar{n}^a\bar{l}^a\,|\,r^a)Z(\bar{n}^b\bar{l}^b\,|\,r^b)j(\bar{L}\,|\,kr)I(\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M}\,|\,RR^aR^b)\\&+\frac{1}{2\pi}\int\cdots\int\Bigg\{\Sigma\left(-\frac{\mu ki}{2\pi\hbar^2}\right)\\&\times\frac{(2l_1+1)(2l_2+1)(2l_5+1)}{8\pi^2}j_{l_5}(kr_<)h_{l_5}(kr_>)\\&\times I(l_1l_2l_3l_5l_4M\,|\,RR^aR^b)J(l_1l_2l_3l_5l_4M\,|\,R'S^{a'}S^{b'})^*\\&\times Z(n_1l_1\,|\,r^a)Z(n_1l_1\,|\,r^a)^*Z(n_2l_2\,|\,r^b)Z(n_2l_2\,|\,r^{b'})^*\\&\times v(\lambda_1\lambda_2u_2\,|\,r'r^{a'}r^{b'})D(\lambda_10-u_2\,|\,S^{a'})\\&\times D(\lambda_20u_2\,|\,S^{b'})\psi(n^{a'}n^{b'}l^{a'}l^{b'}l'\lambda'L'M'\,|\,r')\\&\times Z(n^{a'}l^{a'}\,|\,r^{a'})Z(n^{b'}l^{b'}\,|\,r^{b'})\\&\times J(l^{a'}l^{b'}l'\lambda'L'M'\,|\,R'S^{a'}S^{b'})\Bigg\}\\&\times r'^2dr'dr^{a'}dr^{b'}dR'dS^{a'}dS^{b'},\end{aligned} \tag{3.6}$$

where the sum is over $n_1n_2l_1l_2l_3l_4Mn^{a\prime}n^{b\prime}l^{a\prime}l^{b\prime}\lambda'L'M'\lambda_1\lambda_2\mu_2$, and $\bar{k}$ or k is $k(\bar{n}^a\bar{l}^a\bar{n}^b\bar{l}^b)$ or $k(n_1l_1n_2l_2)$, respectively.

This form of the integral equation can be simplified by use of the orthonormality of the Z's and the orthogonality of the I's,

$$\int\int\int I(l^al^b l\lambda LM|RR^aR^b)$$
$$\times I(l^{a\prime}l^{b\prime}l'\lambda'L'M'|RR^aR^b)^*dRdR^adR^b$$
$$=\delta_{l^al^{a\prime}}\delta_{l^bl^{b\prime}}\delta_{ll'}\delta_{\lambda\lambda'}\delta_{LL'}\delta_{MM'}\frac{(8\pi^2)^3}{(2l^a+1)(2l^b+1)(2\lambda+1)}.$$

Then if the vibrational matrix element be written

$$v(n^al^an^bl^b;\lambda_1\lambda_2\mu_2;n^{a\prime}l^{a\prime}n^{b\prime}l^{b\prime}|r)$$
$$=\int\int Z(n^al^a|r^a)^*Z(n^bl^b|r^b)^*v(\lambda_1\lambda_2\mu_2|rr^ar^b)$$
$$\times Z(n^{a\prime}l^{a\prime}|r^a)Z(n^{b\prime}l^{b\prime}|r^b)dr^adr^b \quad (3.7)$$

and an integral operator be defined

$$G(\lambda n^al^an^bl^b)f(r)$$
$$=\int j_\lambda(k(n^al^an^bl^b)r_<)h_\lambda(k(n^al^an^bl^b)r_>)$$
$$\times r'^2f(r')dr', \quad (3.8)$$

the resulting set of coupled integral equations (an integro-matric equation) becomes [we use $\delta(a,b,\cdots;a',b',\cdots)$ as shorthand for $\delta_{aa'}\delta_{bb'}\cdots$]

$$\psi(n^an^bl^al^bl\lambda LM|r)$$
$$=\delta(n^an^bl^al^bl\lambda LM;\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M})j[\bar{\lambda}|k(\bar{n}^a\bar{l}^a\bar{n}^b\bar{l}^b)]$$
$$+\sum_{\substack{n^{a\prime}n^{b\prime}l^{a\prime}l^{b\prime}\\ l'\lambda'L'M'\\ \lambda_1\lambda_2\mu_2}}\left(-\frac{\mu ki}{4\pi^2\hbar^2}\right)\cdot\frac{(2l^a+1)(2l^b+1)(2\lambda+1)}{(8\pi^2)^2}$$
$$\times\Big[\int\int\int J(l^al^bl\lambda LM|R'S^{a\prime}S^{b\prime})^*$$
$$\times D(\lambda_10-\mu_2|S^{a\prime})D(\lambda_20\mu_2|S^{b\prime})$$
$$\times J(l^{a\prime}l^{b\prime}l'\lambda'L'M'|R'S^{a\prime}S^{b\prime})dR'dS^{a\prime}dS^{b\prime}\Big]$$
$$\times G(\lambda n^al^an^bl^b)\{v(n^al^an^bl^b;\lambda_1\lambda_2\mu_2,n^{a\prime}l^{a\prime}n^{b\prime}l^{b\prime}|r)$$
$$\times\psi(n^{a\prime}n^{b\prime}l^{a\prime}l^{b\prime}l'\lambda'L'M'|r)\}. \quad (3.9)$$

It remains to evaluate the quantity within brackets in Eq. (3.9). Let it be labeled A. Then, on writing the J's in terms of their definition [Eq. (2.8)], we have

$$A=\int\int\int\sum_{sts't'}C(l^al^bl st)C(l\lambda L,s+t,0)D(l^a0s|S^a)^*$$
$$\times D(l^b0t|S^b)^*D(L,s+t,M|R)D(\lambda_10-\mu_2|S^a)$$
$$\times D(\lambda_20\mu_2|S^b)C(l^{a\prime}l^{b\prime}l's't')C(l'\lambda'L',s'+t',0)$$
$$\times D(l^{a\prime}0s'|S^a)D(l^{b\prime}0t'|S^{b\prime})$$
$$\times D(L',s'+t',M'|R)dRdS^adS^b.$$

Now the integral with respect to R is immediately seen to equal

$$\delta_{LL'}\delta_{MM'}\delta_{s+t,s'+t'}[8\pi^2/(2L+1)]$$

by the orthogonality of the representation coefficients. Similarly, integrals over products of three D's can be expressed in terms of the Clebsch-Gordan coefficients, with results that the integral over S^a is

$$\frac{8\pi^2}{2l^a+1}C(l^{a\prime}\lambda_1l^a00)C(l^{a\prime}\lambda_1l^a,s+\mu_2,-\mu_2)\delta_{s',s+\mu_2}$$

and that over S^b is

$$\frac{8\pi^2}{2l^b+1}C(l^{b\prime}\lambda_2l^b00)C(l^{b\prime}\lambda_2l^b,t-\mu_2,\mu_2)\delta t',t-\mu_2.$$

Combining these results leads to

$$A=\frac{(8\pi^2)^3}{(2l^a+1)(2l^b+1)(2L+1)}\delta_{LL'}\delta_{MM'}\sum_{s,t}C(l^al^bl st)$$
$$\times C(l\lambda L,s+t,0)C(l'\lambda'L,s+t,0)$$
$$\times C(l^{a\prime}l^{b\prime}l's+\mu_2,t-\mu_2)C(l^{a\prime}\lambda_1l^a00)$$
$$\times C(l^{a\prime}\lambda_1l^a,s+\mu_2,-\mu_2)C(l^{b\prime}\lambda_2l^b00)$$
$$\times C(l^{b\prime}\lambda_2l^b,t-\mu_2,\mu_2)$$

which, on substitution in Eq. (3.9), yields

$$\psi(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M};n^an^bl^al^bl\lambda LM|r)$$
$$=\delta(n^an^bl^al^bl\lambda LM;\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M})j(\bar{\lambda}|\bar{k}r)$$
$$-\frac{2\mu ki}{\hbar^2}\sum_{\substack{l^{a\prime}l^{b\prime}l'\lambda'\\ \lambda_1\lambda_2\mu_2st}}\left(\frac{2\lambda+1}{2L+1}\right)C(l^al^bl st)C(l^{a\prime}l^{b\prime}l'st)$$
$$\times C(l\lambda L,s+t,0)C(l'\lambda'L',s+t,0)C(l^{a\prime}\lambda_1l^a00)$$
$$\times C(l^{a\prime}\lambda_1l^a,s+\mu_2,-\mu_2)C(l^{b\prime}\lambda_2l^b00)$$
$$\times C(l^{b\prime}\lambda_2l^b,t-\mu_2,\mu_2)G(\lambda n^al^an^bl^b)$$
$$\times\{v(n^al^an^bl^b;\lambda_1\lambda_2\mu_2;n^{a\prime}l^{a\prime}n^{b\prime}l^{b\prime}|r)$$
$$\times\psi(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M};n^{a\prime}n^{b\prime}l^{a\prime}l^{b\prime}l'\lambda'L'M'|r)\}, \quad (3.10)$$

where $k=k(n^al^an^bl^b)$ and $\bar{k}=k(\bar{n}^a\bar{l}^a\bar{n}^b\bar{l}^b)$. It should be

noted that $\delta(L,M;\bar{L},\bar{M})$ occurs in the inhomogeneous term of the integral equation, and there is no mixing among the values of L and M in the homogeneous term. Thus unless $M=\bar{M}$ and $L=\bar{L}$, the equation is homogeneous and can have only zero as a solution. Furthermore, neither M nor $\bar{M}$ appears other than in the unknown ψ, so that ψ is not a function of $\bar{M}$ at all. Symbolically, the foregoing statements are

$$\psi(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M};n^an^bl^al^bl\lambda LM|r)$$
$$=\delta(L,M;\bar{L}\bar{M})\psi(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}0;n^an^bl^al^bl\lambda\bar{L}0). \quad (3.11)$$

It is this simplification which is the purpose of the introduction of initial states of sharp angular momentum, rather than the plane waves one would otherwise prefer.

4. CROSS SECTIONS

The first step in evaluating the collision cross sections is to find a linear combination of the initial states φ used in the previous section which forms a plane wave

$$\varphi_0=e^{i\mathbf{k}\cdot\mathbf{r}}Y(\bar{l}^a\bar{m}^a)Y(\bar{l}^b\bar{m}^b)Z(\bar{n}^a\bar{l}^a)Z(\bar{n}^b\bar{l}^b). \quad (4.1)$$

Given this, the same linear combination of the solutions ψ to the integral equation will form a solution which has a plane wave for its initial state, which is just the sort of solution needed in forming the cross section. Now the initial state given in Eq. (3.2) is already in the form of Eq. (4.1) as far as the vibrational wave functions are concerned, so that these may be ignored in what follows.

The linear combination needed must be of the form

$$e^{i\mathbf{k}\cdot\mathbf{r}}Y(\bar{l}^a\bar{m}^a)Y(\bar{l}^b\bar{m}^b)$$
$$=\sum d(\bar{l}^a\bar{m}^a\bar{l}^b\bar{m}^b;\bar{l}\bar{\lambda}\bar{L}\bar{M})$$
$$\times I(\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}\bar{M}|RR^aR^b)j(\bar{\lambda}|kr), \quad (4.2)$$

where the sum is over $\bar{l}$, $\bar{\lambda}$, $\bar{L}$, and $\bar{M}$. The coefficients d may also be functions of the wave number vector $\mathbf{k}$, or perhaps only its direction as described by the rotation T. It is not difficult to show, by use of Eq. (2.2), that

$$d(\bar{l}^a\bar{m}^a\bar{l}^b\bar{m}^b;\bar{l}\bar{\lambda}\bar{L}\bar{M})$$
$$=[(2\bar{l}^a+1)(2\bar{l}^b+1)]^{\frac{1}{2}}(4\pi)^{-1}i^{M^*}(2\bar{\lambda}+1)$$
$$\times D(\bar{\lambda}0,\bar{m}^a+\bar{m}^b-\bar{M}|T)C(\bar{l}\bar{\lambda}\bar{L},\bar{m}^a+\bar{m}^b,$$
$$\bar{M}-\bar{m}^a-\bar{m}^b)C(\bar{l}^a\bar{l}^b\bar{l}\bar{m}^a\bar{m}^b), \quad (4.3)$$

where $M^*=\bar{\lambda}+2(\bar{M}-\bar{m}^a-\bar{m}^b)$. It is evident that the solution to the integral equation will have an asymptotic form

$$\psi(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}\bar{L}0;n^an^bl^al^bl\lambda\bar{L}0|r)$$
$$-\delta(\bar{n}^a\cdots,n^a\cdots)j(\bar{\lambda}|kr)\sim f(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda};\bar{L};$$
$$n^an^bl^al^bl\lambda)r^{-1}e^{ikr}, \quad (4.4)$$

where f is a constant with respect to r. The asymptotic form of the solution with plane wave initial state leads to

$$f(T|\bar{n}^a\bar{l}^a\bar{n}^b\bar{l}^b\bar{m}^b;n^al^am^an^bl^bm^b|R)$$
$$=\sum(4\pi)[(2l^a+1)(2l^b+1)]^{-\frac{1}{2}}d(\bar{l}^a\bar{m}^a\bar{l}^b\bar{m}^b;\bar{l}\bar{\lambda}\bar{L}\bar{M})$$
$$\times f(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda};\bar{L};n^an^bl^al^bl\lambda)$$
$$\times C(l\lambda L,m^a+m^b,\bar{M}-m^a-m^b)C(l^al^blm^am^b)$$
$$\times D(\lambda0,M-m^a-m^b|R)$$
$$=\sum[(2\bar{l}^a+1)(2\bar{l}^b+1)]^{\frac{1}{2}}[(2l^a+1)(2l^b+1)]^{-\frac{1}{2}}$$
$$\times i^{M^*}(2\bar{\lambda}+1)C(\bar{l}\bar{\lambda}\bar{L},\bar{m}^a+\bar{m}^b,\bar{M}-\bar{m}^a-\bar{m}^b)$$
$$\times C(l\lambda L,m^a+m^b,\bar{M}-m^a-m^b)C(\bar{l}^a\bar{l}^b\bar{l}\bar{m}^a\bar{m}^b)$$
$$\times C(l^al^blm^am^b)f(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda};\bar{L};n^an^bl^al^bl\lambda)$$
$$\times D(\bar{\lambda}0,\bar{m}^a+\bar{m}^b-\bar{M}|T)$$
$$\times D(\lambda0,\bar{M}-m^a-m^b|R), \quad (4.5)$$

where both sums are over $\bar{l}\bar{\lambda}\bar{L}\bar{M}l\lambda$, and the second equation arises from the substitution of Eq. (4.3) in the first.

By analogy with[1] Eq. I-(47), the cross section for scattering from internal states $\bar{n}^a\bar{l}^a\bar{m}^a$ and $\bar{n}^b\bar{l}^b\bar{m}^b$ and direction T to states $n^al^am^a$ and $n^bl^bm^b$ and direction R is given by

$$\sigma(\bar{n}^a\bar{l}^a\bar{m}^a\bar{n}^b\bar{l}^b\bar{m}^b;T|n^al^am^an^bl^bm^b;R)$$
$$=[k(n^al^an^bl^b)]/[k(\bar{n}^a\bar{l}^a\bar{n}^b\bar{l}^b)]$$
$$\times|f(T|\bar{n}^a\bar{l}^a\bar{m}^a\bar{n}^b\bar{l}^b\bar{m}^b;n^al^am^an^bl^bm^b|R)|^2.$$

The absolute square may be written as the product of f with its complex conjugate, and if primed dummy indices are used for the latter, a series over the 12 indices

$$\bar{l}\bar{\lambda}\bar{L}\bar{M}l\lambda\bar{l}'\bar{\lambda}'\bar{L}'\bar{M}'l'\lambda'$$

results. The factor

$$D(\bar{\lambda}0\bar{m}^a+\bar{m}^b-\bar{M}|T)D(\bar{\lambda}'0\bar{m}^a+\bar{m}^b-\bar{M}'|T)^*$$
$$\times D(\lambda0\bar{M}-m^a-m^b|R)D(\lambda'0\bar{M}'-m^a-m^b|R)^*$$

may be transformed by use of the Clebsch-Gordan series to

$$(-1)^{m^a+m^b+\bar{m}^a+\bar{m}^b}\sum_{\lambda_3\lambda_4}C(\bar{\lambda}\bar{\lambda}'\lambda_300)$$
$$\times C(\bar{\lambda}\bar{\lambda}'\lambda_3,\bar{m}^a+\bar{m}^b-\bar{M},\bar{M}'-\bar{m}^a-\bar{m}^b)$$
$$\times D(\lambda_30\bar{M}'-\bar{M}|T)C(\lambda\lambda'\lambda_400)$$
$$\times C(\lambda\lambda'\lambda_4,\bar{M}-m^a-m^b,m^a+m^b-\bar{M}')$$
$$\times D(\lambda_40\bar{M}-\bar{M}'|R).$$

Let the abbreviation $\bar{m}=\bar{m}^a+\bar{m}^b$ and $m=m^a+m^b$ be introduced, and the variables $\bar{M}$, $\bar{M}'$ be changed to $\bar{M}=\mu_3$ and $\bar{M}'=\mu_3-\mu_4$. Then the cross section may be written in the form

$$\sigma(\bar{n}^a\cdots;T|n^a\cdots;R)=\sum\sigma(\bar{n}^a\cdots|\lambda_3\lambda_4\mu_4|n^a\cdots)$$
$$\times D(\lambda_30-\mu_4|T)D(\lambda_40\mu_4|R), \quad (4.6)$$

where

$$\sigma(\bar{n}^a\bar{l}^a\bar{m}^a\bar{n}^b\bar{l}^b\bar{m}^b|\lambda_3\lambda_4\mu_4|n^al^am^an^bl^bm^b)$$
$$=\frac{k(n^al^an^bl^b)}{k(\bar{n}^a\bar{l}^a\bar{n}^b\bar{l}^b)}\cdot\frac{(2\bar{l}^a+1)(2\bar{l}^b+1)}{(2l^a+1)(2l^b+1)}\sum i^{\mu^*}(2\bar{\lambda}'+1)$$
$$\times(2\lambda+1)C(\bar{l}\bar{\lambda}L,\bar{m},\mu_3-\bar{m})C(\bar{l}'\bar{\lambda}'L',\bar{m},\mu_3-\mu_4-\bar{m})$$
$$\times C(\bar{l}^a\bar{l}^b\bar{l}\bar{m}^a\bar{m}^b)C(\bar{l}^a\bar{l}^b\bar{l}'\bar{m}^a\bar{m}^b)C(l^al^bl m^am^b)$$
$$\times C(l^al^bl'm^am^b)C(\bar{\lambda}\bar{\lambda}'\lambda_300)C(\lambda\lambda'\lambda_400)$$
$$\times C(\bar{\lambda}\bar{\lambda}'\lambda_3,\bar{m}-\mu_3,\mu_3-\mu_4-\bar{m})$$
$$\times C(\lambda\lambda'\lambda_4,\mu_3-m,m+\mu_4-\mu_3)$$
$$\times f(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda};L;n^an^bl^al^bl\lambda)$$
$$\times f(\bar{n}^a\bar{n}^b\bar{l}^a\bar{l}^b\bar{l}'\bar{\lambda}';L';n^an^bl^al^bl'\lambda')^*, \quad (4.7)$$

where $\mu^*=\bar{\lambda}-\bar{\lambda}'+2(\mu_4+m+\bar{m})$ and the sum is over $l\bar{l}\bar{\lambda}\lambda l'\bar{l}'\bar{\lambda}'\lambda'LL'\mu_3$. Thus the cross sections, which are the goal of this study, are exhibited explicitly in terms of the solutions of an integral equation.

The form chosen for the presentation of the cross section, as a series in what are essentially spherical harmonics of the initial and final angles, is believed to be quite significant. It is clearly not limited to the case here considered, but rather should hold for any scattering process, since it is a very natural development of the group-theoretical formalism. A similar relation has been given by Blatt and Biedenharn[15] in connection with nuclear scattering, and also by the present authors in connection with a limited approximation.[16] While there is some question of the rapidity of convergence of the series, its use is expected to be extremely valuable in the kinetic theory of gases, since there the cross sections occur as variously weighted angular averages. Thus, by use of the orthogonality relations among the spherical harmonics it would be possible to obviate both the labor and inaccuracy of a numerical integration.

5. CROSS SECTIONS: UNPOLARIZED BEAMS

Many physical systems are such that the distribution among the quantum numbers m^a, m^b is uniform. Such is the case at equilibrium, of course, and may very well remain so at conditions sufficiently near equilibrium. Such would also be the case in a typical molecular beam scattering experiment. Since the cross section is defined as the number of particles per unit solid angle per unit initial flux, the proper average to use in such situations is one averaged over incoming particles and summed over outgoing. On noting that there are $2l+1$ values of m for each l, we define[17]

$$\sigma(\bar{l}^a\bar{l}^b,T|l^al^b,R)=[(2\bar{l}^a+1)(2\bar{l}^b+1)]^{-1}\times\sum\sigma(\bar{l}^a\bar{m}^a\bar{l}^b\bar{m}^b,T|l^am^al^bm^b,R), \quad (5.1)$$

where the sum is over $m^am^b\bar{m}^a\bar{m}^b$. The cross section coefficients $\sigma(\bar{l}^a\cdots|\lambda_3\lambda_4\mu_4|l^a\cdots)$ of Eq. (4.6) are averaged similarly.

Inspection of Eq. (4.7) shows that the indices m as well as the dummy index μ_3 occur only in known factors, either in Clebsch-Gordan coefficients or in exponents. Let the summation be changed to one over m^a and $m=m^a+m^b$. Then the following sum,

$$\sum_{m^a}C(l^al^bl,m^a,m-m^a)C(l^al^bl',m^a,m-m^a)=\delta_{ll'}, \quad (5.2)$$

as well as a similar one over barred indices, is seen to occur. The sum over m leads to a Racah function,

$$\sum_m(-1)^mC(l\lambda L,m,\mu_3-m)C(l\lambda'L',m,\mu_3-m-\mu_4)\times C(\lambda\lambda'\lambda_4,\mu_3-m,m+\mu_4-\mu_3)$$
$$=(-1)^{L'+L+\lambda+\lambda'}[(2L+1)(2L'+1)]^{\frac{1}{2}}\times C(LL'\lambda_4,-\mu_3,\mu_3-\mu_4)W(L\bar{\lambda}L'\bar{\lambda}';\bar{l}\lambda_3), \quad (5.3)$$

while the sum over $\bar{m}$ yields

$$(-1)^{l^*}[(2L+1)(2L'+1)]^{\frac{1}{2}}\times C(LL'\lambda_3,-\mu_3,\mu_3-\mu_4)W(L\bar{\lambda}L'\bar{\lambda}';\bar{l}\lambda_3), \quad (5.4)$$

where $l^*=\bar{l}+\lambda_3+L+L'$. Finally, a sum over μ_3 gives

$$\sum_{\mu_3}C(LL'\lambda_3,-\mu_3,\mu_3-\mu_4)C(LL'\lambda_4,-\mu_3,\mu_3-\mu_4)=\delta_{\lambda_3\lambda_4}. \quad (5.5)$$

In the process of evaluating the sums over m's and μ_3, the index μ_4 no longer appears in any Clebsch-Gordan coefficient. On noting that

$$D(\lambda_3\mu_40|T^{-1})=(-1)^{\mu_4}D(\lambda_30-\mu_4|T),$$

we have that

$$\sum_{\mu_4}(-1)^{\mu_4}D(\lambda_30-\mu_4|T)D(\lambda_30\mu_4|R)=\sum_{\mu_4}D(\lambda_30\mu_4|R)D(\lambda_3\mu_40|T^{-1})=D(\lambda_300|RT^{-1}). \quad (5.6)$$

Combination of Eqs. (5.2–6) yields the following form for the cross section:

$$\sigma(\bar{l}^a\bar{l}^bT|l^al^bR)=\sum_{\lambda_3}\sigma(\bar{l}^a\bar{l}^b;l^al^b|\lambda_3)D(\lambda_300|RT^{-1}), \quad (5.7)$$

[15] J. M. Blatt and L. C. Biedenharn, Revs. Modern Phys. **24**, 249 (1952).

[16] G. Gioumousis and C. F. Curtiss, University of Wisconsin Naval Research Laboratory Rept. OOR-8 (1953).

[17] The vibrational quantum numbers play no role in the considerations of this section and thus need not be written.

where

$$\sigma(\bar{l}^a\bar{l}^b; l^al^b|\lambda_3)$$
$$=[k(l^al^b)/k(\bar{l}^a\bar{l}^b)][(2l^a+1)(2l^b+1)]^{-1}$$
$$\times\sum i^{\lambda^*}(2L+1)(2L'+1)(2\bar{\lambda}+1)(2\bar{\lambda}'+1)$$
$$\times C(\bar{\lambda}\bar{\lambda}'\lambda_3 00)C(\lambda\lambda'\lambda_3 00)W(L\lambda L'\lambda'; l\lambda_3)$$
$$\times W(L\bar{\lambda}L'\bar{\lambda}'; \bar{l}\lambda_3)f(\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}; L; l^al^bl\lambda)$$
$$\times f(\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda}'; L'; l^al^bl\lambda')^*, \quad (5.8)$$

where the sum is over $l\bar{l}\lambda\lambda'\bar{\lambda}LL'$, and $\lambda^*=\bar{\lambda}-\bar{\lambda}'+2(l+\bar{l})$. The virtue of such an averaging procedure, where it is valid, is obvious. Thus Eq. (5.8) is summed over eight indices compared to the 11 in Eq. (4.7), and the sum in Eq. (5.7) is over one index compared to the three in Eq. (4.6). Further, Eq. (5.7) shows that the cross section is now only a function of the angle between the incoming and outgoing directions, and there is no longer any preferred direction in space, which is a reasonable result.

6. CERTAIN SPECIAL CASES

The use of group theory makes it possible to exploit whatever symmetries may exist in any particular problem. As a first example, the effect of the symmetry of the potential will be considered. We discuss in particular the case in which a or b or both are homonuclear, and the case in which a and b are identical.

First consider a rotation R used to specify the direction of a vector $\mathbf{v}$. Let R' be the rotation for the diametrically opposite vector $-\mathbf{v}$. Then it is easily shown that[18]

$$D(l0m|R')=(-1)^lD(l0m|R), \quad (6.1)$$

where it should be noted that these representation coefficients are not functions of the first Eulerian angle, the one which is arbitrary.

Now if both ends of a are the same, the potential energy function, expressed in R, R^a, R^b, is unchanged if R^a is replaced by $R^{a'}$. Thus

$$V(rr^ar^b,R^aR^{-1},R^bR^{-1})=V(rr^ar^b,R^{a'}R^{-1},R^bR^{-1}),$$

or by Eqs. (2.5) and (6.1),

$$\sum_{l_1l_2\mu_2s_1s_2}(-1)^{s_1+s_2}v(l_1l_2\mu_2|rr^ar^b)D(l_10s_1|R^a)$$
$$\times D(l_20s_2|R^b)D(l_1-s_1\mu_2|R)D(l_2-s_2-\mu_2|R)$$
$$=\sum_{l_1l_2\mu_2s_1s_2}(-1)^{s_1+s_2}v(l_1l_2\mu_2|rr^ar^b)(-1)^{l_1}D(l_10s_1|R^a)$$
$$\times D(l_20s_2|R^b)D(l_1-s_1\mu_2|R)D(l_2-s_2-\mu_2|R). \quad (6.2)$$

On comparing terms, it is seen that $v(l_1l_2u_2|\cdots)$ is zero unless l_1 is even. Similarly, if b is homonuclear v is zero unless l_2 is even. There is no restriction on u_2.

The condition on the potential if a and b are the same is

$$V(rr^ar^b,R^aR^{-1},R^bR^{-1})=V(rr^ar^b,R^bR'^{-1},R^aR'^{-1}),$$

which leads to the series

$$V(rr^ar^b,R^aR^{-1},R^bR^{-1})$$
$$=\sum_{l_1l_2\mu_2s_1s_2l_3}(-1)^{s_1+s_2}v(l_1l_2\mu_2|rr^ar^b)D(l_10s_1|R^b)$$
$$\times D(l_20s_2|R^a)C(l_1l_2l_3-s_1-s_2)C(l_1l_2l_3\mu_2-\mu_2)$$
$$\times D(l_30-s_1-s_2|R')$$

by Eq. (2.5) and the Clebsch-Gordan series. The two equations[4,11]

$$D(l_3,0,-s_1-s_2|R')=(-1)^{l_3}D(l_3,0,-s_1-s_2|R)$$

and

$$C(l_1l_2l_3\mu_2-\mu_2)=(-1)^{l_1+l_2+l_3}C(l_1l_2l_3-\mu_2\mu_2)$$

yield, on summing over l_3, a different Clebsch-Gordan series equal to

$$(-1)^{l_1+l_2}D(l_1-\mu_2-s_1|R)D(l_2\mu_2-s_2|R)$$
$$=(-1)^{l_1+l_2}(-1)^{s_1+s_2}D(l_1s_1\mu_2|R^{-1})D(l_2s_2-\mu_2|R^{-1}).$$

Substitution of the above into the equation for V and interchanging the indices l_1 and l_2 yields

$$V(rr^ar^bS^aS^b)=\sum(-1)^{l_1+l_2}v(l_2l_1\mu_2|rr^ar^b)$$
$$\times D(l_20\mu_2|S^b)D(l_10-\mu_2|S^a),$$

which on comparison with Eq. (2.4) yields

$$v(l_1l_2\mu_2|rr^ar^b)=(-1)^{l_1+l_2}v(l_2l_1\mu_2|rr^ar^b)$$

as the condition that the molecules a and b be identical.

In much the same way, it is possible to show that

$$v(l_1l_2\mu_2|rr^ar^b)=v(l_1l_2-\mu_2|rr^ar^b)^*$$

is the condition that the potential is real; it thus must hold in all cases.

These relations show clearly in what ways the form of the potential is limited under various conditions. There are similar restrictions in the number of terms which can appear in the series such as Eqs. (3.10), (4.7), and (5.8), as a result of the triangle condition on the $C(j_1j_2j_3m_1m_2)$, that is, that the coefficient is zero unless[6]

$$|j_1-j_2|\leqslant j_3\leqslant j_1+j_2,$$

and the very similar conditions on the Racah coefficients. Further, the rule that $C(j_1j_2j_300)$ is zero unless $j_1+j_2+j_3$ is even restricts the indices, λ_1 and λ_2 of the matrix element $v(\cdots;\lambda_1\lambda_2\mu_2;\cdots)$ to the same parity as $l^a+l^{a'}$ and $l^b+l^{b'}$ in Eq. (3.10), while a similar restriction holds with respect to $\bar{\lambda}$, $\bar{\lambda}'$, and λ_3, and λ, λ', and λ_3 from Eq. (5.8).

Since examination of special cases is often more enlightening than the perusal of generalities, let us consider the form of Eqs. (3.10) and (5.8) for the evaluation of the cross section coefficients $\sigma(00;02;\lambda_3)$, that is, for a collision in which one molecule remains in its ground state and the other is raised from the ground

[18] G. Gioumousis, University of Wisconsin Naval Research Laboratory Rept. WIS-NSF-5 (1955), p. 135.

to the second excited state. From Eq. (3.10), since $l^a=0$, $l^b=2$ then $l=2$. The second coefficient gives

$$|\lambda-L|\leqslant 2\leqslant\lambda+L$$

and the third and fifth $\lambda_1=l^{a'}$ and $\lambda_2=l^{b'}$, $l^{b'}\pm 1$, respectively.

As mentioned previously, only the first few values of λ_3 in Eq. (5.8) are needed for the application to the kinetic theory of gasses. Apart from a factor of four, the coefficient for $\lambda_3=0$ is the total cross section, and has the simple form

$$\sigma(\bar{l}^a\bar{l}^b;\, l^a l^b|0)=(k/\bar{k})[(2l^a+1)(2l^b+1)]^{-1}\times\sum(2L+1)|f(\bar{l}^a\bar{l}^b\bar{l}\bar{\lambda};\, L;\, l^a l^b l\lambda)|^2,$$

where the sum is over $L\lambda\bar{\lambda}l\bar{l}$. Similarly, for $\lambda_3=1$ the parity rule and the triangle rule impose the restriction $\bar{\lambda}'=\bar{\lambda}\pm 1$ and $\lambda'=\lambda\pm 1$, while for $\lambda_3=2$ the restriction is $\bar{\lambda}'=\bar{\lambda}$, $\bar{\lambda}\pm 2$ and $\lambda'=\lambda$, $\lambda\pm 2$.

Similar selection rules arise in various approximation schemes. Thus to first order approximation (say, the Born approximation, or distorted wave) if only the $\lambda_1=1$, $\lambda_2=1$ terms in the potential are considered the selection rule is $\Delta l^a=0,\ \pm 1$, $\Delta l^b=0,\ \pm 1$. Similarly, if a is homonuclear, by the result following Eq. (6.2) only the even λ_1 give nonzero terms in the potential. Thus, to first order, $\Delta l^a=\pm 1$ is forbidden and $\Delta l^a=0,\ \pm 2$ permitted.

7. CONCLUSION

The work described in this paper has been based on the point of view that the introduction of approximations and simplifying assumptions should be delayed as long as possible. (It is well recognized that such a course also delays one's arrival to the point of numerical results.) Thus the results herein developed, the simplifications attendant on the use of group theory and the expansion of the cross section in spherical harmonics, are valid without significant approximation. It is believed that the problem has been carried as far as conveniently possible in its full generality, so that further work must be based on special cases and simplifying assumptions.

Note added in proof. Since this work was completed, a paper by Arthurs and Dalgarno [Proc. Roy. Soc. (London) **A256**, 540 (1960)] has appeared which covers collisions where one molecule is a rigid rotator and the other spherical. The major difference between their work and ours lies in their use of an incoming beam restricted to the z-axis direction. This, in general, is incorrect, but they restrict themselves to cross sections averaged over m's and for this case [as we show in Eq. (5.8)] the restriction is valid.

Some Nonequilibrium Properties of a Bose System of Hard Spheres at Extremely Low Temperatures*

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The pseudopotential method is used to study a special type of flow for a Bose system of hard spheres. In the first-order approximation, the wave function of the entire system is assumed to be the product of identical single-particle wave functions, which in general are time-dependent. Such a flow is necessarily irrotational, and the single-particle wave function satisfies a Schrödinger equation with a nonlinear self-coupling term. On the basis of this equation of motion, the following properties of the Bose system are discussed: the effect of the rigid wall, the moment of inertia, the compressional wave, and a type of "vortex filament." In the second-order approximation, the wave function of the system is expressed in terms of two functions such that one of them describes the single-particle state suitable for most of the particles while the other one describes the pair excitations. The much more complicated equations of motion are found, but in this approximation the flow is no longer strictly irrotational. The compressional waves are also studied in the second-order approximation.

1. INTRODUCTION

RECENTLY, there has been some interest in the properties of a dilute Bose system of hard spheres, since this system serves as a model of superfluids to a certain extent. By using the grand canonical ensemble and its modification (the x-ensemble), Lee and Yang[1] succeeded in obtaining in great detail the equilibrium properties of such a system. Because of this remarkable theory, the low-density expansions of the thermodynamic functions for this system may be considered to be well understood.

Since the quantum theory of transport phenomena is not nearly as well developed as equilibrium statistical mechanics, much less is known about the nonequilibrium properties of such a system. By using the method of the pseudopotential, Lee and Yang[2] obtained equations of motion for this system starting from the microscopic picture. Their equations of motion give a great deal of insight for many problems, particularly the question of the two sound speeds; however, the question whether the superfluid flow is irrotational is not resolved in their paper. In the derivation of these equations of motion, concepts of classical kinetic theory are used. Alternatively, also from the point of view of the pseudopotential, Lee, Huang, and Yang[3] suggested in an earlier paper that the superfluid flow of a dilute Bose system of hard spheres may be represented as the condensation of a finite fraction of the particles into a single-particle state that may not be an eigenstate of the momentum operator. It is the purpose here to develop in some detail a special case of this alternative, since it has the advantage of not making use of any concept borrowed from classical kinetic theory.

In the special case to be considered, the temperature of the system is assumed to be extremely low so that no average over states need to be considered and that the condensation into a single-particle state is approximately complete. Except in the case of a uniform flow, the velocity of the flow must change from point to point. Since the velocity of the flow is related to the phase of the single-particle wave function, it is thus mandatory to allow for an arbitrary phase variation. Because of the conservation of the number of particles, a nonuniform flow must lead to density variations. It is therefore desirable to generalize the form (57) of footnote reference 3 to a function whose absolute value may not be unity. To illustrate this point, consider the special case of extremely low densities. Here the interaction between the particles may be neglected altogether, and the Schrödinger equation for the system may be solved by separation of the variables. If all particles are in the same single-particle state, then the wave function of the system is the product of identical single-particle wave functions. Furthermore, the single-particle wave function must satisfy the one-particle Schrödinger equation without any potential. This equation admits many solutions, but the only ones with constant absolute magnitudes are those corresponding to plane waves. Therefore, in this approximation as studied in Secs. 2–5, the wave function of the system is assumed to be the product of identical single-particle wave functions $\Phi(\mathbf{r},t)$.

In the case of periodic boundary conditions, the specialization of this first approximation to the lowest stationary state merely yields the unperturbed ground state, i.e., the ground state of the system without hard-sphere interactions. When the method of the pseudopotential is used, it is known[3] that a better approximation to the ground-state wave function may be obtained by allowing excitations into pairs, i.e., by taking into consideration the transitions between two particles both in the zero-momentum state and two particles in non-

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[1] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959); **116**, 25 (1959); **117**, 12, 22, 897 (1960).

[2] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1406 (1959).

[3] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).

zero momentum states of opposite momenta. In the second-order approximation (as studied in Secs. 6–9), the wave function of the system is assumed to take on a somewhat more complicated form so that precisely these transitions are taken into account. The specific form used is given by (6.1) and (6.2), and Sec. 6 is devoted to the development of a formalism dealing with wave functions of this form. In Sec. 7, the formalism is applied to the Bose system of hard spheres to get the equations of motion in the second-order approximation. As expected, the equations of motion are rather complicated. Some of the simple properties of these equations are considered in Sec. 8; the compressional waves are studied in Sec. 9, where the conclusion is reached that there is a difference between a phonon and a compressional wave in the second-order approximation.

The Hamiltonian to be studied may be specified as follows. A system of hard spheres is a collection of N pairwise interacting particles with the Hamiltonian ($\hbar=2m=1$)

$$\sum_{i=1}^{N} p_i^2+\sum_{i<j} V_0(r_{ij}), \tag{1.1}$$

where

$$r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|, \tag{1.2}$$

and

$$V_0(r)=\begin{cases}0 & \text{if } r>a,\\ \infty & \text{if } r\leqslant a.\end{cases} \tag{1.3}$$

Here a is the diameter of the hard spheres, and is also the scattering length. Since nonequilibrium properties are to be discussed, the boundary condition for the confining box remains unspecified for the time being.

According to the method of the pseudopotential of Huang and Yang,[4] the Hamiltonian (1.1) may be replaced in a certain approximation by

$$H'=T+V', \tag{1.4}$$

with

$$T=\sum_i p_i^2, \tag{1.5}$$

and

$$V'=4\pi a\sum_{i\neq j}\delta(\mathbf{r}_i-\mathbf{r}_j)(\partial/\partial r_{ij})r_{ij}. \tag{1.6}$$

Unlike the case of the calculation of the ground-state energy per particle, it is sufficient for the present consideration to use

$$H=T+V, \tag{1.7}$$

where

$$V=4\pi a\sum_{i\neq j}\delta(\mathbf{r}_i-\mathbf{r}_j), \tag{1.8}$$

instead of (1.4). The only difficulty in using H instead of H' is the appearance of a familiar type of divergence. This may be removed by the method described in Sec. 1 of footnote reference 3. Thus H is the Hamiltonian to be studied for a Bose system.

[4] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).

2. EQUATION OF MOTION IN FIRST-ORDER APPROXIMATION

As in all previous treatments of problems of this kind, it is convenient to rewrite the pseudo-Hamiltonian H in the language of quantized fields:

$$T=\int d\mathbf{r}|\nabla\psi(\mathbf{r})|^2, \tag{2.1}$$

and

$$V=4\pi a\int d\mathbf{r}\psi^*(\mathbf{r})^2\psi(\mathbf{r})^2, \tag{2.2}$$

where $\psi(\mathbf{r})$ satisfies the usual commutation rules for a boson field. If the state Φ is normalized by

$$\Omega^{-1}\int d\mathbf{r}|\Phi(\mathbf{r},t)|^2=1, \tag{2.3}$$

where Ω is the volume of the confining box, then the creation and annihilation operators for the state Φ may be defined by

$$\begin{aligned}a_0^*(t)&=\Omega^{-\frac{1}{2}}\int d\mathbf{r}\psi^*(\mathbf{r})\Phi(\mathbf{r},t),\\ a_0(t)&=\Omega^{-\frac{1}{2}}\int d\mathbf{r}\psi(\mathbf{r})\Phi^*(\mathbf{r},t).\end{aligned} \tag{2.4}$$

From (2.3), it follows that $a_0(t)$ and $a_0^*(t)$ satisfy the usual commutation rule for equal times

$$[a_0(t),a_0^*(t)]=1.$$

The parts of ψ^* and ψ corresponding to this one state may be singled out as follows:

$$\begin{aligned}\psi^*(\mathbf{r})&=\psi_0^*(\mathbf{r},t)+\psi_1^*(\mathbf{r},t),\\ \psi(\mathbf{r})&=\psi_0(\mathbf{r},t)+\psi_1(\mathbf{r},t),\end{aligned} \tag{2.5}$$

where

$$\begin{aligned}\psi_0^*(\mathbf{r},t)&=\Omega^{-\frac{1}{2}}a_0^*(t)\Phi^*(\mathbf{r},t),\\ \psi_0(\mathbf{r},t)&=\Omega^{-\frac{1}{2}}a_0(t)\Phi(\mathbf{r},t).\end{aligned} \tag{2.6}$$

In the Schrödinger picture, $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$ are time independent, but ψ_0^*, ψ_0, ψ_1^*, and ψ_1 all may depend on the time.

In the equilibrium theory of Lee, Huang, and Yang,[3] the choice is made that $\Phi(\mathbf{r},t)=1$. Then a_0^* and a_0 are considered to be in some sense large compared with the creation and annihilation operators for other single-particle momentum states. For the same reason, in the present procedure ψ_0^* and ψ_0 are considered to be large compared with ψ_1^* and ψ_1. With (2.5) substituted in the Hamiltonian or in any other operator, terms may be classified according to the numbers of times ψ_1^* and ψ_1 appear. As a first approximation only terms of zeroth order or first order in ψ_1^* and ψ_1 are to be kept. Even quadratic terms are dropped. Thus, for example, the

total number of particles is given by

$$N=\int d\mathbf{r}\psi^*(\mathbf{r})\psi(\mathbf{r})$$
$$=a_0^*(t)a_0(t)+\int d\mathbf{r}\psi_1^*(\mathbf{r})\psi_1(\mathbf{r}). \quad (2.7)$$

For the first-order approximation, (2.7) is simply reduced to

$$N\sim a_0^*(t)a_0(t). \quad (2.8)$$

Note that time-independent operators may become time dependent in this approximation. Similarly, the kinetic energy T is approximated by

$$T\sim a_0^*(t)a_0(t)\bar{\zeta}(t)-\Omega^{-\frac{1}{2}}a_0(t)\int d\mathbf{r}\psi_1^*(\mathbf{r},t)\nabla^2\Phi(\mathbf{r},t)$$
$$-\Omega^{-\frac{1}{2}}a_0^*(t)\int d\mathbf{r}\psi_1(\mathbf{r},t)\nabla^2\Phi^*(\mathbf{r},t), \quad (2.9)$$

where

$$\bar{\zeta}(t)=\Omega^{-1}\int d\mathbf{r}|\nabla\Phi(\mathbf{r},t)|^2\geqslant 0. \quad (2.10)$$

Attention has been restricted to those boundary conditions for which the integration by parts does not yield a surface term. The same procedure of approximation may be applied to the V of (2.2) to yield

$$V\sim 4\pi a\Omega^{-1}a_0^*(t)^2a_0(t)^2\zeta(t)$$
$$+8\pi a\Omega^{-\frac{3}{2}}a_0^*(t)a_0(t)^2\int d\mathbf{r}\psi_1^*(\mathbf{r},t)|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t)$$
$$+8\pi a\Omega^{-\frac{3}{2}}a_0^*(t)^2a_0(t)\int d\mathbf{r}\psi_1(\mathbf{r},t)|\Phi(\mathbf{r},t)|^2\Phi^*(\mathbf{r},t), \quad (2.11)$$

where

$$\zeta(t)=\Omega^{-1}\int d\mathbf{r}|\Phi(\mathbf{r},t)|^4\geqslant 1. \quad (2.12)$$

When (2.8) is used in (2.9) and (2.11), the results are called T_1 and V_1, indicating first-order approximation

$$T_1=N\bar{\zeta}(t)-\Omega^{-\frac{1}{2}}a_0(t)\int d\mathbf{r}\psi_1^*(\mathbf{r},t)\nabla^2\Phi(\mathbf{r},t)$$
$$-\Omega^{-\frac{1}{2}}a_0^*(t)\int d\mathbf{r}\psi_1(\mathbf{r},t)\nabla^2\Phi^*(\mathbf{r},t), \quad (2.13)$$

and

$$V_1=4\pi a\rho_0\Big[N\zeta(t)+2\Omega^{-\frac{1}{2}}a_0(t)\int d\mathbf{r}\psi_1^*(\mathbf{r},t)|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t)$$
$$+2\Omega^{-\frac{1}{2}}a_0^*(t)\int d\mathbf{r}\psi_1(\mathbf{r},t)|\Phi(\mathbf{r},t)|^2\Phi^*(\mathbf{r},t)\Big], \quad (2.14)$$

where

$$\rho_0=N/\Omega \quad (2.15)$$

is the average or equilibrium density of the system.

The Hamiltonian

$$H^{(1)}=T_1+V_1 \quad (2.16)$$

is to be studied in the Schrödinger picture, because generalizations seem to be simpler to carry out in this picture. Since $H^{(1)}$ is linear in ψ_1, it is possible to have a Schrödinger state vector of the form

$$\Psi(t)=(N!)^{-\frac{1}{2}}a_0^*(t)^N|\text{vac}\rangle, \quad (2.17)$$

where $|\text{vac}\rangle$ is the state defined by

$$\psi(\mathbf{r})|\text{vac}\rangle=0 \quad (2.18)$$

for all $\mathbf{r}$. The state vector $\Psi(t)$ satisfies the Schrödinger equation

$$H^{(1)}\Psi(t)=i(\partial/\partial t)\Psi(t). \quad (2.19)$$

As shown in Appendix A, this implies the following equation of motion for $a_0^*(t)$:

$$i(\partial/\partial t)a_0^*(t)=[H^{(1)},a_0^*(t)]+[\bar{\zeta}(t)+4\pi a\rho_0\zeta(t)]a_0^*(t). \quad (2.20)$$

This in turn implies an equation of motion for $\Phi(\mathbf{r},t)$:

$$i(\partial/\partial t)\Phi(\mathbf{r},t)=[-\nabla^2+8\pi a\rho_0|\Phi(\mathbf{r},t)|^2$$
$$-4\pi a\rho_0\zeta(t)]\Phi(\mathbf{r},t). \quad (2.21)$$

As may be expected, this equation is in the form of a Schrödinger equation with a self-coupling term of third order. Note that the normalization (2.3) is consistant with (2.21).

3. SOME SIMPLE PROPERTIES OF THE EQUATION OF MOTION IN FIRST-ORDER APPROXIMATION

A. Interpretation

When Φ is written in the form

$$\Phi(\mathbf{r},t)=A(\mathbf{r},t)\exp[i\phi(\mathbf{r},t)], \quad (3.1)$$

the velocity of the fluid may be defined by

$$\mathbf{v}(\mathbf{r},t)=2\nabla\phi(\mathbf{r},t), \quad (3.2)$$

while the number density of the fluid is

$$\rho(\mathbf{r},t)=\rho_0A(\mathbf{r},t)^2. \quad (3.3)$$

The normalization (2.3) gives

$$\int d\mathbf{r}\,\rho(\mathbf{r},t)=N, \quad (3.4)$$

which justifies the term "number density." In terms of A and $\mathbf{v}$, the imaginary and real parts of the equation of motion (2.21) give, respectively,

$$\partial\rho/\partial t+\nabla\cdot(\rho\mathbf{v})=0, \quad (3.5)$$

and

$$\rho[\partial \mathbf{v}/\partial t+(\mathbf{v}\cdot\nabla)\mathbf{v}]=-\nabla(8\pi a\rho^2)+2\rho\nabla(\rho^{-\frac{1}{2}}\nabla^2\rho^{\frac{1}{2}}). \quad (3.6)$$

Equation (3.5) is the usual equation of continuity. Since the mass of each particle has been taken to be $\frac{1}{2}$, the mass density ρ_m is $\frac{1}{2}\rho$. Furthermore, the static pressure at absolute zero is known to be[3]

$$p=4\pi a\rho^2. \quad (3.7)$$

Thus (3.6) is equivalent to

$$\rho_m D\mathbf{v}/Dt=-\nabla p+2\rho_m\nabla(\rho_m^{-\frac{1}{2}}\nabla^2\rho_m^{\frac{1}{2}}), \quad (3.8)$$

where D/Dt denotes Lagrangian derivative. Equation (3.2) implies that

$$\nabla\times\mathbf{v}(\mathbf{r},t)=0. \quad (3.9)$$

Except for the last term in (3.8), the Eqs. (3.5), (3.8), and (3.9) are the usual hydrodynamic equations for a superfluid[5] in the absence of normal fluid. Note, however, that (3.9) means that the fluid motion is irrotational in the present case. Since the present approach concerns a very special case of superfluid flow, the question whether superfluid motion can be rotational in general is not touched upon.

B. One-Dimensional Problem in Steady State

Since it is a nonlinear differential equation, (2.21) can be explicitly integrated only in very special cases. In the steady state, the one-dimensional problem is governed by

$$[d^2/dx^2-8\pi a\rho_0|\Phi(x)|^2+4\pi a\rho_0\zeta+E]\Phi(x)=0. \quad (3.10)$$

For a periodic box, the solutions are simply $\exp(ikx)$ with the corresponding energy $k^2+4\pi a\rho_0$. This is in agreement with the results of Lee, Huang, and Yang.[3,6] Therefore, for periodic boundary conditions, it is admissible to use unperturbed wave functions, but take the extra energy $4\pi a\rho_0$ per particle into account.

Equation (3.10) can also be solved with rigid walls at 0 and L. In this case the boundary conditions are

$$\Phi(0)=\Phi(L)=0. \quad (3.11)$$

It then follows from the equation of continuity (3.5) that

$$v(x)=0. \quad (3.12)$$

Without loss of generality, $\Phi(x)$ can be taken to be real. Moreover, the energy of the nth eigenstate of (3.10) for the length L is the same as the ground-state energy for the length L/n, and the eigenfunctions are very simply related. Therefore, it is sufficient to consider the ground state only. For this state (3.11) may be replaced by

$$\Phi(0)=0 \quad \text{and} \quad \partial\Phi/\partial x|_{x=L/2}=0. \quad (3.13)$$

The lowest eigenfunction is thus given by

$$\Phi(x)=\Phi(L/2)\ \mathrm{sn}[2xK(k)/L], \quad (3.14)$$

where sn is the elliptic sine function of modulus k, $\Phi(L/2)$ is given by

$$\Phi(L/2)=(\pi a\rho_0)^{-\frac{1}{2}}kK(k)/L, \quad (3.15)$$

and k is determined by

$$K(k)[K(k)-E(k)]=\pi a\rho_0 L^2. \quad (3.16)$$

Here $K(k)$ and $E(k)$ are complete elliptic integrals of the first and second kinds, respectively. From this solution it is found that

$$\zeta=(3k^2)^{-1}\Phi(L/2)^2[2(1+k^2)-\Phi(L/2)^2], \quad (3.17)$$

and

$$E=4\pi a\rho_0(3k^2)^{-1}\Phi(L/2)^2[1+k^2+\Phi(L/2)^2]. \quad (3.18)$$

It is a simple matter to evaluate these formulas in the limits of large and small L. The results are

$$\begin{aligned} L\gg(a\rho_0)^{-\frac{1}{2}}:\quad & k=1-8\exp[-(4\pi a\rho_0)^{\frac{1}{2}}L], \\ & \Phi(L/2)=1+(4\pi a\rho_0)^{-\frac{1}{2}}L^{-1}, \\ & \zeta=1+\tfrac{4}{3}(4\pi a\rho_0)^{-\frac{1}{2}}L^{-1}, \\ & E=4\pi a\rho_0[1+(8/3)(4\pi a\rho_0)^{-\frac{1}{2}}L^{-1}], \end{aligned} \quad (3.19)$$

and

$$\Phi(x)=\tanh(4\pi a\rho_0)^{\frac{1}{2}}x \quad \text{for } 0\leqslant x\leqslant L/2.$$

$$\begin{aligned} L\ll(a\rho_0)^{-\frac{1}{2}}:\quad & k=(8\pi a\rho_0)^{\frac{1}{2}}L/\pi, \\ & \zeta=\tfrac{3}{2} \\ & E=(\pi/L)^2+6\pi a\rho_0, \end{aligned} \quad (3.20)$$

and

$$\Phi(x)=\sqrt{2}\sin(\pi x/L).$$

C. Question of Rigid Boundaries

The correlation length at absolute zero is defined by[3]

$$r_0=(8\pi a\rho_0)^{-\frac{1}{2}}. \quad (3.21)$$

According to (3.19), when $L\gg r_0$, $\Phi(x)$ differs significantly from 1 only when x or $L-x$ is of the order of r_0. Therefore, for a simply connected region with a smooth rigid boundary such that all radii of curvature are much larger than the correlation length, the lowest eigenfunction is given approximately by

$$\Phi(\mathbf{r})=\tanh[(4\pi a\rho_0)^{\frac{1}{2}}r_{\min}], \quad (3.22)$$

where $r_{\min}$ is the minimum distance from $\mathbf{r}$ to the rigid boundary.

Equation (3.22) implies that the distribution of density is approximately constant in the confining box except within about one correlation length of the rigid boundary. In particular, the wave function is quite different from the unperturbed wave function corresponding to $a=0$, in which case the correlation length is infinite. This point has been emphasized by Lee, Huang, and Yang,[3] and is explicitly demonstrated here.

[5] F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II, pp. 129–130.

[6] T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958).

On the other hand, as seen from (3.2) for the one-dimensional problem, $\Phi(x)$ is approximately independent of a when $L \ll r_0$. In general, this may be expected to be true if a is so small that the correlation length is much larger than all macroscopic dimensions of the confining box.

This consideration may be used to explain the paradox of Eyges,[7] who obtained the following formula for the ground-state energy per particle:

$$E(\text{Eyges}) = (27/4)\pi a\rho_0 \tag{3.23}$$

for the case of the rigid boundary. This is in apparent contradiction with the earlier result $4\pi a\rho_0$ of Huang and Yang.[4] The explanation is that, with rigid walls, $4\pi a\rho_0$ holds for a fixed low density ρ_0 but $N \to \infty$, while the result (3.23) is valid under the condition of very large correlation length or

$$N \ll \Omega^{\frac{1}{3}}/a. \tag{3.24}$$

There can thus be no overlap in the ranges of validity.

The problem of flow in a large pipe with a smooth rigid wall may be studied by applying a Galilean transformation to (3.22). If the pipe is parallel to the x axis, the velocity and density profiles are approximately

$$v_x = v_{x0}$$

and

$$\rho = \rho_0\{\tanh[(4\pi a\rho_0)^{\frac{1}{2}} r_{\min}]\}^2. \tag{3.25}$$

These profiles are quite different from those for the flow of water, say, at low Reynold's numbers.

4. ROTATING BUCKET

In this section, the moment of inertia of a Bose system is to be considered on the basis of (2.21). The correlation length is assumed to be small compared with the macroscopic dimensions of the confining box; thus the noninteracting case with $a=0$ is not included. The wall of the confining box, or the bucket, is assumed to be rigid. Let this rigid boundary be represented by an external potential V_e. If it rotates uniformly with the angular speed ω, then

$$V_e = V_e(r, \theta-\omega t, z), \tag{4.1}$$

where the axis of rotation is chosen to be the z axis for the cylindrical coordinate system. According to (2.21), the equation of motion is

$$i(\partial/\partial t)\Phi(r,\theta,z;t) = [-\nabla^2 + 8\pi a\rho_0|\Phi(r,\theta,z;t)|^2 - 4\pi a\rho_0\zeta(t) + V_e(r,\theta-\omega t,z)]\Phi(r,\theta,z;t). \tag{4.2}$$

The canonical transformation to the rotating coordinate system is

$$\Phi(r,\theta,z;t) = \exp(-i\omega t p_\theta)\Phi_1(r,\theta,z;t) = \Phi_1(r,\theta-\omega t,z;t). \tag{4.3}$$

[7] L. Eyges, Ann. Phys. **2**, 101 (1957). The author is unable to verify Eyges' result, and gets instead an energy larger by a factor of two.

In terms of Φ_1, (4.2) becomes

$$i(\partial/\partial t - \omega\partial/\partial\theta)\Phi_1(r,\theta,z;t) = [-\nabla^2 + 8\pi a\rho_0|\Phi_1(r,\theta,z;t)|^2 - 4\pi a\rho_0\zeta(t) + V_e(r,\theta,z)]\Phi_1(r,\theta,z;t). \tag{4.4}$$

Therefore, in the case of the cylindrical rigid boundary, the time-independent problem is governed by

$$(\lambda - i\omega\partial/\partial\theta)\Phi_1(r,\theta) = [-\nabla^2 + 8\pi a\rho_0|\Phi_1(r,\theta)|^2 - 4\pi a\rho_0\zeta]\Phi_1(r,\theta), \tag{4.5}$$

with the condition on the boundary S

$$\Phi_1 = 0. \tag{4.6}$$

Note that λ is the energy in the rotating system, while the expectation value of the energy in the fixed system is

$$E = \langle\Phi|[-\nabla^2 + 8\pi a\rho_0|\Phi|^2 - 4\pi a\rho_0\zeta]|\Phi\rangle = \bar{\xi} + 4\pi a\rho_0\zeta, \tag{4.7}$$

where $\bar{\xi}$ is defined by (2.10).

Similar to (3.1), let

$$\Phi_1(r,\theta) = A_1(r,\theta)\exp[i\phi_1(r,\theta)]. \tag{4.8}$$

Then the imaginary and real parts of (4.5) give, respectively,

$$A_1\nabla^2\phi_1 + 2\nabla A_1\cdot\nabla\phi_1 = \omega\partial A_1/\partial\theta, \tag{4.9}$$

and

$$-\nabla^2 A_1 + A_1|\nabla\phi_1|^2 + 8\pi a\rho_0 A_1^3 - 4\pi a\rho_0\zeta A_1 = \lambda A_1 + \omega A_1\partial\phi_1/\partial\theta. \tag{4.10}$$

From (3.12), the velocity is everywhere zero in the one-dimensional problem with stationary rigid walls. By a Galilean transformation, the velocity is the same as that of the walls for translational motion. Therefore, for the present problem of the rotating bucket, the normal component of the fluid velocity at the wall is given by

$$2\partial\phi_1/\partial n = v_n \tag{4.11}$$

on S, where v_n is the normal component of the wall velocity. If $\mathbf{n}$ is the unit outward normal, and $\boldsymbol{\theta}$ is the unit vector in the θ direction, then

$$v_n = \omega r\boldsymbol{\theta}\cdot\mathbf{n}. \tag{4.12}$$

When ω is not too large, the fluid density $\rho_0 A_1^2$ is not expected to vary greatly over one correlation length, except near S. Therefore, except near S, A_1 and ϕ_1 may be obtained correctly after neglecting the term $-\nabla^2 A_1$ in (4.10). However, with this approximation, the boundary condition (4.6) cannot be satisfied, and (4.11) may be used in its place. In other words, the functions A_1 and ϕ_1 are to be determined, except an additive constant for ϕ_1, by (4.9) and

$$|\nabla\phi_1|^2 + 8\pi a\rho_0 A_1^2 - 4\pi a\rho_0\zeta = \lambda + \omega\partial\phi_1/\partial\theta \tag{4.13}$$

with

$$\partial\phi_1/\partial n = \tfrac{1}{2}\omega r\boldsymbol{\theta}\cdot\mathbf{n} \tag{4.14}$$

on S.

Attention is now restricted to the case of extremely small ω. In this case, the appropriate expansions are

$$\begin{aligned} A_1&=1+\omega^2 A_2+O(\omega^4),\\ \phi_1&=\omega\phi_2+O(\omega^3),\\ \zeta&=1+O(\omega^4),\\ \lambda&=4\pi a\rho_0+\omega^2\lambda_2+O(\omega^4), \end{aligned} \tag{4.15}$$

and

$$\bar{\zeta}=\omega^2\bar{\zeta}_2+O(\omega^4).$$

The moment of inertia per particle I in the limit $\omega\rightarrow 0$ may be defined by

$$E=4\pi a\rho_0+\tfrac{1}{2}\omega^2 I+O(\omega^4). \tag{4.16}$$

With (4.15), (4.9) and (4.13) become

$$\nabla^2\phi_2=0 \tag{4.17}$$

and

$$A_2=(16\pi a\rho_0)^{-1}[\lambda_2-|\nabla\phi_2|^2+\partial\phi_2/\partial\theta], \tag{4.18}$$

where λ_2 is determined by the normalization

$$\int d\mathbf{r}A_2=0. \tag{4.19}$$

The boundary condition on S

$$\partial\phi_2/\partial n=\tfrac{1}{2}r\boldsymbol{\theta}\cdot\mathbf{n} \tag{4.20}$$

then yields the results

$$\bar{\zeta}_2=-\lambda_2=\tfrac{1}{2}I=\Omega^{-1}\int d\mathbf{r}|\nabla\phi_2|^2=\tfrac{1}{2}\Omega^{-1}\int d\mathbf{r}\partial\phi_2/\partial\theta. \tag{4.21}$$

As usual, the moment of inertia can be decomposed into that of the center of mass and the moment of inertia about the center of mass. To see this, let $\mathbf{R}$ be the position vector of the center of mass, (r',θ') be a cylindrical coordinate system about the center of mass, so that

$$\mathbf{r}'=\mathbf{r}-\mathbf{R} \tag{4.22}$$

and

$$\int d\mathbf{r}\mathbf{r}'=0. \tag{4.23}$$

If ϕ_2' is defined by

$$\nabla^2\phi_2'=0 \quad\text{and}\quad \partial\phi_2'/\partial n=\tfrac{1}{2}r'\boldsymbol{\theta}'\cdot\mathbf{n} \tag{4.24}$$

on S, then the difference is

$$\phi_2-\phi_2'=\tfrac{1}{2}R\boldsymbol{\Theta}\cdot\mathbf{r}_2, \tag{4.25}$$

where $\boldsymbol{\Theta}$ is the unit vector at $\mathbf{R}$ in the θ direction. It is now a consequence of (4.23) that

$$\begin{aligned} I&=I_0+2\Omega^{-1}\int d\mathbf{r}|\nabla(\phi_2-\phi_2')|^2\\ &=I_0+\tfrac{1}{2}R^2, \end{aligned} \tag{4.26}$$

where

$$I_0=2\Omega^{-1}\int d\mathbf{r}|\nabla\phi_2'|^2 \tag{4.27}$$

is the moment of inertia per particle about the center of mass. Equation (4.26) is the desired result; note that the mass of each particle has been taken as $\frac{1}{2}$.

Unlike the case of the rigid body, the moment of inertia here depends very much on the shape of the confining box. For example, the moment of inertia I about the center of mass is zero when the particles are confined in a circular cylinder, but is approximately $[(4/\pi^2)-\frac{1}{4}-(\pi^2/128)]L^2$ when confined in a half-circular cylinder of radius L. It may be of some interest to consider the following model of the circular cylinder with a rough wall. With the complex variable

$$w=re^{i\theta}, \tag{4.28}$$

consider the conformal mapping

$$w=L(z+Cz^n). \tag{4.29}$$

In this particular model, the interior of the rough circular cylinder of radius L is defined to be the set such that $|z|<1$. Here the following conditions are imposed on C and n:

$$1\gg C\gg(a\rho_0L^2)^{-\frac{1}{2}},\quad n\gg 1. \tag{4.30}$$

For this definition of the model to be meaningful, it is necessary that the analytic function $w(z)$ be univalent in the open disk $|z|<1$. This imposes the condition

$$Cn\leqslant 1. \tag{4.31}$$

The calculation of the moment of inertia in this case is now a straightforward exercise in complex variable. The result is

$$I=\tfrac{1}{2}C^2L^2n. \tag{4.32}$$

If a thickness t_r is defined to represent the thickness of the layer following the wall,

$$I=\tfrac{1}{2}L^2(2t_r/L), \tag{4.33}$$

then

$$t_r=\tfrac{1}{2}C^2Ln. \tag{4.34}$$

This is of the order of magnitude of the amplitude of the ripples CL on the boundary under the conditions of (4.30) and (4.31). The bulk of the liquid does not follow the rotational motion.

5. LINEARIZED EQUATION IN FIRST-ORDER APPROXIMATION

A. Linearization

Let $\Phi_0(\mathbf{r},t)$ be a solution of (2.21), and

$$\Phi(\mathbf{r},t)=\Phi_0(\mathbf{r},t)+\epsilon\Phi_1(\mathbf{r},t), \tag{5.1}$$

where Φ and Φ_0 are normalized according to (2.3), and ϵ is a very small real number. It follows from the nor-

malization that

$$\mathrm{Re}\,\Omega^{-1}\int\Phi_0(\mathbf{r},t)\Phi_1^*(\mathbf{r},t)d\mathbf{r}=0. \tag{5.2}$$

If Φ also satisfies (2.21), then Φ_1 satisfies

$$i\partial\Phi_1/\partial t=-\nabla^2\Phi_1+8\pi a\rho_0(2|\Phi_0|^2\Phi_1+\Phi_0^2\Phi_1^*) -4\pi a\rho_0\zeta_0\Phi_1-4\pi a\rho_0\zeta_1\Phi_0, \tag{5.3}$$

where ζ_0 is the ζ for Φ_0 and

$$\zeta_1=4\Omega^{-1}\,\mathrm{Re}\int d\mathbf{r}|\Phi_0|^2\Phi_0\Phi_1^*. \tag{5.4}$$

Equation (5.3) is to be referred to as the linearized equation.

It is sometimes convenient to recast the linearized equation in a slightly different form by defining f and g as follows:

$$\Phi_1(\mathbf{r},t)=\Phi_0(\mathbf{r},t)[f(\mathbf{r},t)+ig(\mathbf{r},t)]. \tag{5.5}$$

If

$$\Phi_0(\mathbf{r},t)=A_0(\mathbf{r},t)\,\exp[i\phi_0(\mathbf{r},t)], \tag{5.6}$$

then

$$\partial f/\partial t=-2A_0^{-1}\nabla A_0\cdot\nabla g-2\nabla\phi_0\cdot\nabla f-\nabla^2 g,$$
$$\partial g/\partial t=2A_0^{-1}\nabla A_0\cdot\nabla f-2\nabla\phi_0\cdot\nabla g+\nabla^2 f -16\pi a\rho_0A_0^2f+4\pi a\rho_0\zeta_1. \tag{5.7}$$

B. Plane Wave

In the special case $A_0=1$, it follows from (2.21) that ϕ_0 satisfies

$$\nabla^2\phi_0=0 \tag{5.8}$$

and

$$\partial\phi_0/\partial t=-|\nabla\phi_0|^2-4\pi a\rho_0. \tag{5.9}$$

With (5.8), the Laplacian of (5.9) gives

$$|\nabla\nabla\phi_0|^2=0. \tag{5.10}$$

Thus, it follows from (5.9) and (5.10) that

$$\phi_0=-(4\pi a\rho_0+|\mathbf{k}|^2)t+\mathbf{k}\cdot\mathbf{r}, \tag{5.11}$$

where $\mathbf{k}$ is a constant vector. By a Galilean transformation, $\mathbf{k}$ may be made zero. In this case, the two forms (5.3) and (5.7) of the linearized equation are

$$i\partial\Phi_1/\partial t=-\nabla^2\Phi_1+8\pi a\rho_0(2\Phi_1+\Phi_1^*)-4\pi a\rho_0\Phi_1, \tag{5.12}$$

and

$$\partial f/\partial t=\nabla^2 g,\quad \partial g/\partial t=\nabla^2 f-16\pi a\rho_0 f. \tag{5.13}$$

It is seen from these equations that the normalization for Φ_1 does not change with t if and only if

$$\mathrm{Im}\int d\mathbf{r}\Phi_1(\mathbf{r},t)^2=0, \tag{5.14}$$

or

$$\int d\mathbf{r}f(\mathbf{r},t)g(\mathbf{r},t)=0. \tag{5.15}$$

A special solution of (5.13) is obtained by assuming

$$f=\cos(\omega t-\mathbf{k}\cdot\mathbf{r}). \tag{5.16}$$

In this case, the relation between ω and $\mathbf{k}$ is

$$\omega=k(k^2+16\pi a\rho_0)^{\frac{1}{4}}. \tag{5.17}$$

This is in agreement with the phonon spectrum of Lee, Huang, and Yang.[8] Indeed, in this case, the solution $\Phi(\mathbf{r},t)$ represents a sinusoidal variation of density and hence a sound wave in the ordinary sense. Moreover, in this very special case (5.15) is satisfied.

C. Cylindrical Wave

Consider a circular cylinder of radius L. Let Φ_0 be given by the right-hand member of (3.22), where it is assumed that L is much larger than the correlation length. The boundary condition for Φ_1 is then in the form that f and g are finite at $r=L$. By an argument used in Sec. 4, the approximation

$$A_0(\mathbf{r},t)=1 \tag{5.18}$$

is used and the boundary condition is replaced by

$$\partial f/\partial r=\partial g/\partial r=0 \tag{5.19}$$

at $r=L$. In this approximation, (5.13) is valid. If the angular dependence of f and g are assumed to be of the form $e^{i\theta}$, then (5.13) becomes

$$\partial f/\partial t=-(\partial^2/\partial r^2+r^{-1}\partial/\partial r-r^{-2})g,$$
$$\partial g/\partial t=(\partial^2/\partial r^2+r^{-1}\partial/\partial r-r^{-2}-16\pi a\rho_0)f. \tag{5.20}$$

The corresponding eigenvalue problem in terms of f alone is

$$(\partial^2/\partial r^2+r^{-1}\partial/\partial r-r^{-2}) \times(\partial^2/\partial r^2+r^{-1}\partial/\partial r-r^{-2}-16\pi a\rho_0)f=\omega^2 f. \tag{5.21}$$

With (5.19), the solution of this eigenvalue problem is approximately

$$\{[\omega^2+(8\pi a\rho_0)^2]^{\frac{1}{2}}-8\pi a\rho_0\}^{\frac{1}{2}}L=J_{11}', \tag{5.22}$$

where J_{11}' is the first zero of J_1'. Thus

$$\omega=(16\pi a\rho_0)^{\frac{1}{4}}J_{11}'/L. \tag{5.23}$$

This is to be contrasted with the noninteracting case $a=0$, where the energy is proportional to L^{-2}.

There seems to be some similarity between the present solution and the vortex filament of Onsager[8] and Feynman.[9]

6. FORMALISM FOR SECOND-ORDER APPROXIMATION

A. State Vector

When the system of bosons is in the lowest stationary state in a box with periodic boundary conditions, all the

[8] L. Onsager, Nuovo cimento Suppl. **6**, 249 (1949).
[9] R. P. Feynman, Progr. Low Temp. Phys. **1**, 17 (1955).

results obtained so far become trivial in the sense that the wave function is independent of the scattering length a except in a phase factor. It has been shown by Lee, Huang, and Yang[3] that in this case of the ground state the major effect of the interaction on the wave function is the creation and annihilation of pairs of opposite momenta. In the second-order approximation, a modification is made to include just this effect. In this section, a possible formalism is presented to achieve just this purpose. The Hamiltonian is assumed to a polynomial functional of $\psi(\mathbf{r})$ and $\psi^*(\mathbf{r})$ such that it commutes with the number operator N. No specific form of the Hamiltonian is used. In the next section, this formalism is applied to the Hamiltonian (1.7) to get the second-order equations of motion for a dilute Bose system of hard spheres.

Since the creation and annihilation of pairs are the important processes, it is assumed that the state vector (2.17) is modified in this approximation, to be

$$\Psi(t)=\mathfrak{N}(t)e^{P(t)}(N!)^{-\frac{1}{2}}a_0^*(t)^N|\text{vac}\rangle, \tag{6.1}$$

where $P(t)$ describes the creation of pairs

$$P(t)=[2N_0(t)]^{-1}\int d\mathbf{r}d\mathbf{r}'\psi_1^*(\mathbf{r},t)\psi_1^*(\mathbf{r}',t) \times K_0(\mathbf{r},\mathbf{r}';t)a_0(t)^2. \tag{6.2}$$

Here $N_0(t)$ is the expected number of particles in the state $\Phi(\mathbf{r},t)$

$$N_0(t)=\Omega\rho_1(t)=\langle\Psi(t)|a_0^*(t)a_0(t)|\Psi(t)\rangle. \tag{6.3}$$

In the following, when there is no confusion, the variable t will not be written explicitly. Without loss of generality, it is possible to choose the K_0 of (6.2) such that

$$K_0(\mathbf{r}',\mathbf{r})=K_0(\mathbf{r},\mathbf{r}'), \tag{6.4}$$

and

$$\int d\mathbf{r}\Phi^*(\mathbf{r})K_0(\mathbf{r},\mathbf{r}')=0. \tag{6.5}$$

The case of the lowest stationary state is discussed in Appendix B.

Since P describes the creation of a pair, it is further assumed that the pair created does not consist of two excitations very far apart. In other words, the assumption is made that $K_0(\mathbf{r}',\mathbf{r})$ is substantially different from zero only when $|\mathbf{r}'-\mathbf{r}|$ is not much larger than a characteristic distance, which in turn is much smaller than any macroscopic dimension of the confining box.

Since the state vector Ψ is normalized, the normalization $\mathfrak{N}$ is given by

$$\mathfrak{N}^{-2}=(N!)^{-1}\langle\text{vac}|a_0^N(\exp P^*)(\exp P)a_0^{*N}|\text{vac}\rangle. \tag{6.6}$$

This is evaluated in Appendix C. It is useful to define the following functions:

$$W_1(\mathbf{r}',\mathbf{r})=\int d\mathbf{r}''K_0^*(\mathbf{r}',\mathbf{r}'')K_0(\mathbf{r}'',\mathbf{r}); \tag{6.7}$$

$$W_n(\mathbf{r}',\mathbf{r})=\int d\mathbf{r}''W_1(\mathbf{r}',\mathbf{r}'')W_{n-1}(\mathbf{r}'',\mathbf{r}) =\int d\mathbf{r}''W_{n-1}(\mathbf{r}',\mathbf{r}'')W_1(\mathbf{r}'',\mathbf{r}) \tag{6.8}$$

for $n\geqslant 2$;

$$K_n(\mathbf{r}',\mathbf{r})=K_n(\mathbf{r},\mathbf{r}')=\int d\mathbf{r}''K_0(\mathbf{r}',\mathbf{r}'')W_n(\mathbf{r}'',\mathbf{r}) =\int d\mathbf{r}''K_{n-1}(\mathbf{r}',\mathbf{r}'')W_1(\mathbf{r}'',\mathbf{r}) \tag{6.9}$$

for $n\geqslant 1$;

$$W(\mathbf{r}',\mathbf{r})=\sum_{n=1}^{\infty}W_n(\mathbf{r}',\mathbf{r}); \tag{6.10}$$

$$\tilde{W}(\mathbf{r}',\mathbf{r})=\delta(\mathbf{r}'-\mathbf{r})+W(\mathbf{r}',\mathbf{r}); \tag{6.11}$$

$$\tilde{W}'(\mathbf{r}',\mathbf{r})=\tilde{W}(\mathbf{r}',\mathbf{r})-\Omega^{-1}\Phi^*(\mathbf{r}')\Phi(\mathbf{r}); \tag{6.12}$$

$$K(\mathbf{r}',\mathbf{r})=\sum_{n=0}^{\infty}K_n(\mathbf{r}',\mathbf{r}); \tag{6.13}$$

$$\bar{W}_n=\Omega^{-1}\int d\mathbf{r}W_n(\mathbf{r},\mathbf{r}); \tag{6.14}$$

and

$$\bar{W}=\sum_{n=1}^{\infty}\bar{W}_n=\Omega^{-1}\int d\mathbf{r}W(\mathbf{r},\mathbf{r}). \tag{6.15}$$

In terms of $\bar{W}_n$, $\mathfrak{N}$ is given by

$$\mathfrak{N}^{-2}=\left[1+\rho_0^{-1}\sum_{n=1}^{\infty}(2n+1)\bar{W}_n\right]^{-\frac{1}{2}} \times\exp\left[N\left(\log\frac{N}{N_0}+\frac{N}{N_0}-1+\frac{1}{2\rho_0}\bar{W}\right)\right]. \tag{6.16}$$

With (6.16), the following rule for finding the expectation value of an operator may be formulated.

Rule A (discussed in Appendix C): Consider the operator

$$S=\phi_1(\mathbf{r}_1)\phi_1(\mathbf{r}_2)\phi_1(\mathbf{r}_3)\cdots\phi_1(\mathbf{r}_{2n})a_0^{*\alpha}a_0^{\beta}, \tag{6.17}$$

where each ϕ_1 is either ψ_1 or ψ_1^*, and the numbers α and β are related so that $[S,N]=0$. Carry out the following procedure:

(i) Group $\mathbf{r}_1,\cdots\mathbf{r}_{2n}$ into n pairs. The first member of the pair always has a smaller index than the second member.

(ii) Make the following substitutions for each of the

pairs $(\mathbf{r}_i,\mathbf{r}_j)$

$$\psi_1^*(\mathbf{r}_i)\psi_1(\mathbf{r}_j)\rightarrow W(\mathbf{r}_i,\mathbf{r}_j),$$
$$\psi_1(\mathbf{r}_i)\psi_1^*(\mathbf{r}_j)\rightarrow \tilde{W}'(\mathbf{r}_j,\mathbf{r}_i),$$
$$\psi_1(\mathbf{r}_i)\psi_1(\mathbf{r}_j)\rightarrow K(\mathbf{r}_i,\mathbf{r}_j), \tag{6.18}$$

and

$$\psi_1^*(\mathbf{r}_i)\psi_1^*(\mathbf{r}_j)\rightarrow K^*(\mathbf{r}_i,\mathbf{r}_j).$$

(iii) Substitute

$$a_0\rightarrow N_0^{\frac{1}{2}},\quad a_0^*\rightarrow N_0^{\frac{1}{2}}.$$

This gives a numerical function of $\mathbf{r}_1\cdots\mathbf{r}_{2n}$.

(iv) Sum over all distinct groupings. The result is an approximate formula for $\langle\Psi|S|\Psi\rangle$.

In connection with the equation of motion, the following rule is also useful.

Rule B (discussed in Appendix D): Consider the operators

$$S_1=S(\mathbf{r}_1,\cdots\mathbf{r}_{2n};\alpha,\beta),$$

and

$$S_2=S(\mathbf{r}_1'\cdots\mathbf{r}_{2n'}';\alpha',\beta'),$$

such that $[S_1,N]=[S_2,N]=0$. Carry out the following procedure:

(i) Form $S_3=S(\mathbf{r}_1,\cdots\mathbf{r}_{2n},\mathbf{r}_1',\cdots\mathbf{r}_{2n'}';\alpha+\alpha',\beta+\beta')$.

(ii) Carry out the steps A(i)–(iii) for S_3.

(iii) Sum over all groupings with at least one pair of the form $(\mathbf{r}_i,\mathbf{r}_j')$.

The result is an approximate formula for

$$\langle\Psi|S_1S_2|\Psi\rangle-\langle\Psi|S_1|\Psi\rangle\langle\Psi|S_2|\Psi\rangle.$$

In Appendix E, some properties of a number-distribution function are discussed.

B. Variation of the State Vector

With (6.1) and (6.16), the change of the state vector may be expressed in terms of the corresponding changes in Φ and K_0. Let a subscript t be used to denote time derivative, e.g.,

$$K_{0t}(\mathbf{r}',\mathbf{r})=(\partial/\partial t)K_0(\mathbf{r}',\mathbf{r})=(\partial/\partial t)K_0(\mathbf{r}',\mathbf{r};t). \tag{6.19}$$

It follows from (2.3), (6.4), and (6.5) that

$$\Omega^{-1}\int d\mathbf{r}\Phi_t(\mathbf{r})\Phi^*(\mathbf{r})=iB, \tag{6.20}$$

where B is a real number,

$$K_{0t}(\mathbf{r}',\mathbf{r})=K_{0t}(\mathbf{r},\mathbf{r}'), \tag{6.21}$$

and

$$\int d\mathbf{r}'\Phi^*(\mathbf{r}')K_{0t}(\mathbf{r}',\mathbf{r})=-\int d\mathbf{r}'\Phi_t^*(\mathbf{r}')K_0(\mathbf{r}',\mathbf{r})=M(\mathbf{r}). \tag{6.22}$$

Equation (6.22) defines $M(\mathbf{r})$. Moreover,

$$\int d\mathbf{r}\Phi^*(\mathbf{r})M(\mathbf{r})=0. \tag{6.23}$$

Φ_t and K_{0t} induce variations in N_0, $\mathfrak{N}$, and P. These are given by

$$N_{0t}=-\Omega d\bar{W}/dt, \tag{6.24}$$

$$\mathfrak{N}_t/\mathfrak{N}=\tfrac{1}{2}\Omega\bar{W}N_{0t}/N_0 -\tfrac{1}{2}\,\mathrm{Re}\int d\mathbf{r}d\mathbf{r}'K_{0t}(\mathbf{r}',\mathbf{r})K^*(\mathbf{r},\mathbf{r}'), \tag{6.25}$$

and

$$P_t=-(N_{0t}/N_0)P +(2N_0)^{-1}\int d\mathbf{r}d\mathbf{r}'\psi^*(\mathbf{r})\psi^*(\mathbf{r}')K_{0t}(\mathbf{r},\mathbf{r}')a_0^2 +N_0^{-1}\int d\mathbf{r}d\mathbf{r}'\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')K_0(\mathbf{r},\mathbf{r}')a_0a_{0t}. \tag{6.26}$$

From (6.26), the time derivative of e^P may be computed by

$$(d/dt)e^P=e^P\{P_t+\tfrac{1}{2}[P_t,P]\}, \tag{6.27}$$

because

$$\{[P_t,P],P\}=0. \tag{6.28}$$

Let Q be the operator that contains only ψ_1^* and a_0, and that satisfies

$$iQa_0^{*N}|\mathrm{vac}\rangle=\{\mathfrak{N}_t/\mathfrak{N}+P_t+\tfrac{1}{2}[P_t,P]\}a_0^{*N}|\mathrm{vac}\rangle +Na_{0t}^*a_0^{*N-1}|\mathrm{vac}\rangle; \tag{6.29}$$

then

$$\Psi_t=iQ\Psi. \tag{6.30}$$

Explicitly

$$Q=Q_0+Q_1, \tag{6.31}$$

where

$$Q_0=NB-i\mathfrak{N}_t/\mathfrak{N}-(2N_0)^{-1}\int d\mathbf{r}d\mathbf{r}'\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}') \times[iK_{0t}(\mathbf{r},\mathbf{r}')+(2B-iN_{0t}/N_0)K_0(\mathbf{r},\mathbf{r}')]a_0^2, \tag{6.32}$$

and

$$Q_1=-i\Omega^{-\frac{1}{2}}\int d\mathbf{r}\psi_1^*(\mathbf{r}) \times[\Phi_t(\mathbf{r})+N_0^{-1}(N-2P)M(\mathbf{r})]a_0. \tag{6.33}$$

Note that Q_0 is an even functional of $\psi_1^*(\mathbf{r})$, while Q_1 is an odd functional. Finally, it follows from rule A, (6.24) and (6.31) that

$$\langle\Psi|Q_0|\Psi\rangle=N_0B+\tfrac{1}{2}\,\mathrm{Im}\int d\mathbf{r}d\mathbf{r}'K_{0t}(\mathbf{r}',\mathbf{r})K^*(\mathbf{r},\mathbf{r}'), \tag{6.34}$$

which is real.

C. Variational Principle

Consider the Schrödinger equation

$$i(\partial/\partial t)\Psi_0(t)=H\Psi_0(t), \tag{6.35}$$

with the initial condition $\Psi_0(0)=\Psi_0$, which is given by (B1). Because of the creation of triplets, the matrix element $\langle\Psi_0(t)|\Psi_0\rangle$ approaches zero exceedingly rapidly as t deviates from zero. Nevertheless, the pair state $\Psi_0\exp[-itE_0]$, where E_0 is the ground state energy, is a useful approximation to $\Psi_0(t)$. In the more general nonequilibrium case here considered, it is assumed that the situation is still so fortunate, i.e., there is for all t a useful approximation to the state vector in the form of the $\Psi(t)$ of (6.1).

Under this assumption, the equations of motion for Φ and K may be found as follows. Let δt be an infinitesimal time increment, Φ_t and K_t are to be determined by maximizing the quantity.

$$\langle\Psi(t+\delta t)|e^{-iH\delta t}|\Psi(t)\rangle,$$

under the constraint

$$\langle\Psi(t+\delta t)|\Psi(t+\delta t)\rangle=\langle\Psi(t)|\Psi(t)\rangle=1. \tag{6.36}$$

Again omitting the variable t, the expansion

$$\Psi(t+\delta t)=\Psi+\Psi_t\delta t+\tfrac{1}{2}\Psi_{tt}(\delta t)^2 \tag{6.37}$$

yields the approximation

$$\begin{aligned}\langle\Psi(t+\delta t)|e^{-iH\delta t}|\Psi(t)\rangle&\\ =1+\delta t(\langle\Psi_t|\Psi\rangle+\langle\Psi|-iH|\Psi\rangle)&\\ +\tfrac{1}{2}(\delta t)^2(\langle\Psi_{tt}|\Psi\rangle+2\langle\Psi_t|-iH|\Psi\rangle-\langle\Psi|H^2|\Psi\rangle).&\end{aligned} \tag{6.38}$$

Equation (6.36) implies that

$$\langle\Psi_t|\Psi\rangle+\langle\Psi|\Psi_t\rangle=0. \tag{6.39}$$

Accordingly, the coefficient of δt in (6.38) is imaginary and hence must vanish,

$$i\langle\Psi_t|\Psi\rangle+\langle\Psi|H|\Psi\rangle=0. \tag{6.40}$$

The imaginary part of the coefficient of $(\delta t)^2$ in (6.38) is just

$$-\tfrac{1}{4}(\partial/\partial t)(i\langle\Psi_t|\Psi\rangle-i\langle\Psi|\Psi_t\rangle+2\langle\Psi|H|\Psi\rangle),$$

which also vanishes by (6.40). With

$$\langle\Psi_{tt}|\Psi\rangle+2\langle\Psi_t|\Psi_t\rangle+\langle\Psi|\Psi_{tt}\rangle=0, \tag{6.41}$$

(6.38) reduces to

$$\langle\Psi(t+\delta t)|e^{-iH\delta t}|\Psi(t)\rangle=1-\tfrac{1}{2}(\delta t)^2J, \tag{6.42}$$

where

$$\begin{aligned}J=\langle\Psi_t|\Psi_t\rangle+i\langle\Psi_t|H|\Psi\rangle-i\langle\Psi|H|\Psi_t\rangle&\\ +\langle\Psi|H^2|\Psi\rangle.&\end{aligned} \tag{6.43}$$

The prescription to find the equations of motion is thus to minimize J under the constraint (6.40).

When Ψ_t is expressed by (6.30), J becomes

$$J=\langle\Psi|(Q^*+H)(Q+H)|\Psi\rangle \tag{6.44}$$

and (6.40) is simply

$$\langle\Psi|(Q+H)|\Psi\rangle=0. \tag{6.45}$$

D. Properties of J

Since invariance under space-coordinate translation has been preserved in the entire discussion, conservation of linear momentum follows immediately under appropriate boundary conditions. It remains to discuss the conservation of energy, and for this purpose it is advantageous to obtain certain properties of J first. These properties are also useful in the next section.

Because of rule B, it is more convenient to minimize J in the form

$$\begin{aligned}J=\langle\Psi|(Q^*+H)(Q+H)|\Psi\rangle&\\ -\langle\Psi|(Q^*+H)|\Psi\rangle\langle\Psi|(Q+H)|\Psi\rangle.&\end{aligned} \tag{6.46}$$

By analogy with (6.31), write H in the form

$$H=H_0+H_1, \tag{6.47}$$

where H_0 is an even functional of $\Psi_1^*(\mathbf{r})$ and $\Psi_1(\mathbf{r})$ and H_1 is an odd functional of $\Psi_1^*(\mathbf{r})$ and $\Psi_1(\mathbf{r})$. Clearly

$$\langle\Psi|H_1|\Psi\rangle=\langle\Psi|Q_1|\Psi\rangle=0.$$

Thus the J of (6.46) may be written as

$$\begin{aligned}J=\langle\Psi|(Q_0^*+H_0)(Q_0+H_0)|\Psi\rangle&\\ -\langle\Psi|(Q_0^*+H_0)|\Psi\rangle\langle\Psi|(Q_0+H_0)|\Psi\rangle&\\ +\langle\Psi|(Q_1^*+H_1)(Q_1+H_1)|\Psi\rangle.&\end{aligned} \tag{6.48}$$

Since the constraint

$$\langle\Psi|(Q_0+H_0)|\Psi\rangle=0 \tag{6.49}$$

may be considered merely as the condition for the determination of B, the prescription for obtaining the equations of motion in the second-order approximation is just to minimize J.

The last term on the right-hand side of (6.48) is to be evaluated by rule A. For this purpose, the P in the Q_1 of (6.33) may be replaced by its expectation value

$$\langle\Psi|P|\Psi\rangle=\tfrac{1}{2}\Omega\bar{W}. \tag{6.50}$$

Thus, by (C17) Q_1 reduces to

$$Q_1=i\Omega^{-\frac{1}{2}}\int d\mathbf{r}\psi_1^*(\mathbf{r})F_1(\mathbf{r})a_0, \tag{6.51}$$

where

$$F_1(\mathbf{r})=\Phi_t(\mathbf{r})+M(\mathbf{r}). \tag{6.52}$$

Similarly, it is convenient to write

$$\begin{aligned}Q_0=NB-i\mathfrak{N}_t/\mathfrak{N}&\\ -(2N_0)^{-1}i\int d\mathbf{r}d\mathbf{r}'\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')F_2(\mathbf{r},\mathbf{r}')a_0^2,&\end{aligned} \tag{6.53}$$

where

$$F_2(\mathbf{r},\mathbf{r}')=F_2(\mathbf{r}',\mathbf{r})$$
$$=K_{0t}(\mathbf{r}',\mathbf{r})-(2iB+N_{0t}/N_0)K_0(\mathbf{r}',\mathbf{r}). \quad (6.54)$$

The equations of motion are to be obtained from

$$\delta J/\delta F_1(\mathbf{r})=0 \quad (6.55)$$

and

$$\delta J/\delta F_2(\mathbf{r},\mathbf{r}')=0. \quad (6.56)$$

In computing the variational derivatives, F_1, F_1^*, F_2, and F_2^* are to be considered to be independent functions.

By rules A and B, the substitution of (6.51) and (6.53) into (6.48) gives

$$J=\rho_1\int d\mathbf{r}d\mathbf{r}'F_1(\mathbf{r})F_1^*(\mathbf{r}')\tilde{W}'(\mathbf{r},\mathbf{r}')$$
$$+\tfrac{1}{2}\int d\mathbf{r}d\mathbf{r}'d\mathbf{r}''d\mathbf{r}'''F_2(\mathbf{r},\mathbf{r}')F_2^*(\mathbf{r}'',\mathbf{r}''')$$
$$\times\tilde{W}'(\mathbf{r},\mathbf{r}'')\tilde{W}'(\mathbf{r}',\mathbf{r}''')$$
$$-i\rho_1\int d\mathbf{r}F_1(\mathbf{r})G_1(\mathbf{r})+i\rho_1\int d\mathbf{r}F_1^*(\mathbf{r})G_1^*(\mathbf{r})$$
$$-i\tfrac{1}{2}\int d\mathbf{r}d\mathbf{r}'F_2(\mathbf{r},\mathbf{r}')G_2(\mathbf{r},\mathbf{r}')$$
$$+i\tfrac{1}{2}\int d\mathbf{r}d\mathbf{r}'F_2^*(\mathbf{r},\mathbf{r}')G_2^*(\mathbf{r},\mathbf{r}')+J_0, \quad (6.57)$$

where

$$G_1(\mathbf{r})=N_0^{-1}\Omega^{\frac{1}{2}}\langle\Psi|H_1\psi_1^*(\mathbf{r})a_0|\Psi\rangle, \quad (6.58)$$

$$G_2(\mathbf{r},\mathbf{r}')=\langle\Psi|H_0\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')|\Psi\rangle$$
$$-\langle\Psi|H_0|\Psi\rangle\langle\Psi|\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')|\Psi\rangle, \quad (6.59)$$

and

$$J_0=\langle\Psi|H^2|\Psi\rangle-\langle\Psi|H|\Psi\rangle^2. \quad (6.60)$$

Equations (6.55) and (6.56) then give, respectively,

$$\int d\mathbf{r}'F_1(\mathbf{r}')\tilde{W}'(\mathbf{r}',\mathbf{r})=-iG_1^*(\mathbf{r}), \quad (6.61)$$

and

$$\int d\mathbf{r}''d\mathbf{r}'''F_2(\mathbf{r}'',\mathbf{r}''')\tilde{W}'(\mathbf{r}'',\mathbf{r})\tilde{W}'(\mathbf{r}''',\mathbf{r}')$$
$$=-iG_2^*(\mathbf{r},\mathbf{r}'). \quad (6.62)$$

Equations (6.61) and (6.62) give explicitly G_1 and G_2 in terms of F_1 and F_2. In particular, they lead to

$$\langle\Psi|H_0Q_0|\Psi\rangle-\langle\Psi|H_0|\Psi\rangle\langle\Psi|Q_0|\Psi\rangle$$
$$=-\tfrac{1}{2}\int d\mathbf{r}d\mathbf{r}'d\mathbf{r}''d\mathbf{r}'''F_2(\mathbf{r},\mathbf{r}')F_2^*(\mathbf{r}'',\mathbf{r}''')$$
$$\times\tilde{W}'(\mathbf{r},\mathbf{r}'')\tilde{W}'(\mathbf{r}',\mathbf{r}''') \quad (6.63)$$

and

$$\langle\Psi|H_1Q_1|\Psi\rangle=-\rho_1\int d\mathbf{r}d\mathbf{r}'F_1(\mathbf{r})F_1^*(\mathbf{r}')\tilde{W}'(\mathbf{r},\mathbf{r}'). \quad (6.64)$$

This shows explicitly that $\langle\Psi|HQ|\Psi\rangle$ is real because of (6.49); or with (6.30)

$$(d/dt)\langle\Psi|H|\Psi\rangle=-\operatorname{Im}\langle\Psi|HQ|\Psi\rangle=0. \quad (6.65)$$

This is the conservation of energy.

In order to study further (6.61) and (6.62), it is convenient to introduce the projection operator $\mathcal{P}$ to the space orthogonal to Φ, i.e.,

$$\mathcal{P}f(\mathbf{r})=\int d\mathbf{r}'f(\mathbf{r}')[\delta(\mathbf{r}'-\mathbf{r})-\Omega^{-1}\Phi^*(\mathbf{r}')\Phi(\mathbf{r})]. \quad (6.66)$$

It is easy to verify that

$$\int d\mathbf{r}'\tilde{W}'(\mathbf{r}'',\mathbf{r}')[\delta(\mathbf{r}'-\mathbf{r})-W_1(\mathbf{r}',\mathbf{r})]=\mathcal{P}\delta(\mathbf{r}''-\mathbf{r}). \quad (6.67)$$

Application of (6.67) to (6.61) and (6.62) yields

$$\mathcal{P}F_1(\mathbf{r})=-i\int d\mathbf{r}'G_1^*(\mathbf{r}')[\delta(\mathbf{r}'-\mathbf{r})-W_1(\mathbf{r}',\mathbf{r})], \quad (6.68)$$

and

$$\mathcal{P}\mathcal{P}'F_2(\mathbf{r},\mathbf{r}')=-i\int d\mathbf{r}''d\mathbf{r}'''G_2^*(\mathbf{r}'',\mathbf{r}''')$$
$$\times[\delta(\mathbf{r}''-\mathbf{r})-W_1(\mathbf{r}'',\mathbf{r})]$$
$$\times[\delta(\mathbf{r}'''-\mathbf{r}')-W_1(\mathbf{r}''',\mathbf{r}')]. \quad (6.69)$$

The formalism will not be carried any further; instead, attention is directed to the special case of the Hamiltonian as given by (1.7).

7. EQUATIONS OF MOTION IN SECOND-ORDER APPROXIMATION

The various terms of the Hamiltonian are classified in order of magnitude according to the number of times ψ_1^* and ψ_1 appear. In the first-order approximation, only terms with none or with one of the operators ψ_1^* or ψ_1 are kept. For the second-order approximation, it is necessary first to determine which terms to keep. For the case of the ground state, an appropriate parameter of expansion is $(\rho_0a^3)^{\frac{1}{2}}$, at least for the first few orders of approximation. On the other hand, for the ground state, the depletion factor, which contains one ψ_1^* and one ψ_1, is of the order of magnitude $(\rho_0a^3)^{\frac{1}{2}}$. It is therefore natural to consider two of the operators ψ_1^* or ψ_1 to correspond to one extra lower order of magnitude. Therefore, for the second-order approximation, it is necessary to keep terms that include up to three of the operators ψ_1^* or ψ_1.

To save some writing, let c.c. denote the Hermitian conjugate of the previous term. From (2.2), V in this

approximation takes the form

$$V\sim 4\pi a\Omega^{-1}\zeta a_0^{*2}a_0^2$$
$$+8\pi a\Omega^{-\frac{1}{2}}a_0^*a_0^2\int d\mathbf{r}\psi_1^*(r)\Phi(\mathbf{r})|\Phi(\mathbf{r})|^2+\text{c.c.}$$
$$+16\pi a\Omega^{-1}a_0^*a_0\int d\mathbf{r}\psi_1^*(\mathbf{r})\psi_1(\mathbf{r})|\Phi(\mathbf{r})|^2$$
$$+4\pi a\Omega^{-1}a_0^2\int d\mathbf{r}\psi_1^*(\mathbf{r})^2\Phi(\mathbf{r})^2+\text{c.c.}$$
$$+8\pi a\Omega^{-\frac{1}{2}}a_0\int d\mathbf{r}\psi_1^*(\mathbf{r})^2\psi_1(\mathbf{r})\Phi(\mathbf{r})+\text{c.c.} \quad (7.1)$$

In view of a previous calculation,[10] no term corresponding to a three-body pseudopotential is included in (7.1) for the present case of hard spheres. If the basic two-body interaction is of a different form, such a three-body pseudopotential may be necessary. With the Hamiltonian split in the form (6.47), the second-order approximations to H_0 and H_1 are, respectively,

$$H_0=N_0(\bar{\xi}+4\pi a\rho_1\zeta)-\eta(\bar{\xi}+8\pi a\rho_1\zeta)$$
$$+\int d\mathbf{r}\psi_1^*(\mathbf{r})[-\nabla^2+16\pi a\rho_1|\Phi(\mathbf{r})|^2]\psi_1(\mathbf{r})$$
$$+4\pi a\Omega^{-1}a_0^{*2}\int d\mathbf{r}\psi_1(\mathbf{r})^2\Phi^*(\mathbf{r})^2+\text{c.c.}, \quad (7.2)$$

and

$$H_1=\int d\mathbf{r}\psi_1^*(\mathbf{r})[-\nabla^2+8\pi a\rho_1|\Phi(\mathbf{r})|^2-8\pi a\Omega^{-1}\eta|\Phi(\mathbf{r})|^2$$
$$+8\pi a\psi_1^*(\mathbf{r})\psi_1(\mathbf{r})]\Phi(\mathbf{r})a_0\Omega^{-\frac{1}{2}}+\text{c.c.}, \quad (7.3)$$

where

$$\eta=N_0-N+\int d\mathbf{r}\psi_1^*(\mathbf{r})\psi_1(\mathbf{r}). \quad (7.4)$$

The entire formalism of the last section may now be applied. In particular, (6.68) is explicitly

$$\mathcal{P}F_1(\mathbf{r})=-i\mathcal{P}\Theta(\mathbf{r})-i\int d\mathbf{r}'K_0(\mathbf{r}',\mathbf{r})\Theta^*(\mathbf{r}'), \quad (7.5)$$

where

$$\Theta(\mathbf{r})=[-\nabla^2+8\pi a\rho_1|\Phi(\mathbf{r})|^2+16\pi aW(\mathbf{r},\mathbf{r})]\Phi(\mathbf{r})$$
$$+8\pi aK(\mathbf{r},\mathbf{r})\Phi^*(\mathbf{r}); \quad (7.6)$$

while (6.69) is

$$\mathcal{P}\mathcal{P}'F_2(\mathbf{r},\mathbf{r}')$$
$$=-i\mathcal{P}\mathcal{P}'\Big\{[-\nabla^2-\nabla'^2+16\pi a\rho_1|\Phi(\mathbf{r})|^2$$
$$+16\pi a\rho_1|\Phi(\mathbf{r}')|^2-2\bar{\xi}-16\pi a\rho_1\zeta]K_0(\mathbf{r},\mathbf{r}')$$
$$+8\pi a\rho_1\Phi(\mathbf{r})^2\delta(\mathbf{r}'-\mathbf{r})$$
$$+8\pi a\rho_1\int d\mathbf{r}''K_0(\mathbf{r},\mathbf{r}'')K_0(\mathbf{r}',\mathbf{r}'')\Phi^*(\mathbf{r}'')^2\Big\}. \quad (7.7)$$

By (6.22) and the results of Appendix E, (7.5) is equivalent to

$$\mathcal{P}[\Phi_t(\mathbf{r})+i\Theta(\mathbf{r})]=0. \quad (7.8)$$

The other projections of Φ_t and K_{0t} may be easily found from (6.5), (6.20), and (6.22):

$$(1-\mathcal{P})K_{0t}(\mathbf{r},\mathbf{r}')=\Omega^{-1}\Phi(\mathbf{r})M(\mathbf{r}'); \quad (7.9)$$
$$(1-\mathcal{P}')K_{0t}(\mathbf{r},\mathbf{r}')=\Omega^{-1}M(\mathbf{r})\Phi(\mathbf{r}'); \quad (7.10)$$
$$(1-\mathcal{P})(1-\mathcal{P}')K_{0t}(\mathbf{r},\mathbf{r}')=0; \quad (7.11)$$

and

$$(1-\mathcal{P})\Phi_t(\mathbf{r})=iB\Phi(\mathbf{r}). \quad (7.12)$$

Equations (7.7)–(7.12) finally give the desired equations of motion in the second-order approximation:

$$iK_{0t}(\mathbf{r},\mathbf{r}')=-(2B-iN_{0t}/N_0)K_0(\mathbf{r},\mathbf{r}')$$
$$+[-\nabla^2-\nabla'^2+16\pi a\rho_1|\Phi(\mathbf{r})|^2$$
$$+16\pi a\rho_1|\Phi(\mathbf{r}')|^2-2\bar{\xi}-16\pi a\rho_1]K_0(\mathbf{r},\mathbf{r}')$$
$$+8\pi a\rho_1\Phi(\mathbf{r})^2\delta(\mathbf{r}-\mathbf{r}')$$
$$+8\pi a\rho_1\int d\mathbf{r}''K_0(\mathbf{r},\mathbf{r}'')K_0(\mathbf{r}',\mathbf{r}'')\Phi^*(\mathbf{r}'')^2$$
$$-\Phi(\mathbf{r})\Lambda(\mathbf{r}')-\Phi(\mathbf{r}')\Lambda(\mathbf{r}), \quad (7.13)$$

and

$$i\Phi_t(\mathbf{r})=-B'\Phi(\mathbf{r})+[-\nabla^2+8\pi a\rho_1|\Phi(\mathbf{r})|^2$$
$$+16\pi aW(\mathbf{r},\mathbf{r})]\Phi(\mathbf{r})+8\pi aK(\mathbf{r},\mathbf{r})\Phi^*(\mathbf{r}), \quad (7.14)$$

where

$$\Lambda(\mathbf{r})=8\pi a\rho_1\Omega^{-1}[(|\Phi(\mathbf{r})|^2-\tfrac{1}{2}\zeta)\Phi(\mathbf{r})$$
$$+\int d\mathbf{r}'K_0(\mathbf{r},\mathbf{r}')\Phi^*(\mathbf{r}')|\Phi(\mathbf{r}')|^2, \quad (7.15)$$

and

$$B'=B+\bar{\xi}+8\pi a\rho_1\zeta+16\pi a\Omega^{-1}\int d\mathbf{r}W(\mathbf{r},\mathbf{r})|\Phi(\mathbf{r})|^2$$
$$+8\pi a\Omega^{-1}\int d\mathbf{r}K(\mathbf{r},\mathbf{r})\Phi^*(\mathbf{r})^2. \quad (7.16)$$

It only remains to obtain an explicit formula for B from (6.49), using (6.34), (7.2), and rule A:

$$B=-\bar{\xi}-4\pi a\rho_1\zeta-(2N_0)^{-1}\,\mathrm{Im}\int d\mathbf{r}d\mathbf{r}'K_{0t}(\mathbf{r},\mathbf{r}')K^*(\mathbf{r}',\mathbf{r})$$
$$-N_0^{-1}8\pi a\rho_1\,\mathrm{Re}\int d\mathbf{r}K(\mathbf{r},\mathbf{r})\Phi^*(\mathbf{r})^2$$
$$-N_0^{-1}\int d\mathbf{r}\{[-\nabla^2+16\pi a\rho_1|\Phi(\mathbf{r})|^2]W(\mathbf{r}',\mathbf{r})\}_{\mathbf{r}'=\mathbf{r}}, \quad (7.17)$$

[10] T. T. Wu, Phys. Rev. **115**, 1390 (1959).

so that

$$B'=4\pi a\rho_1\zeta-(2N_0)^{-1}\,\mathrm{Im}\int d\mathbf{r}d\mathbf{r}'K_{0t}(\mathbf{r},\mathbf{r}')K^*(\mathbf{r}',\mathbf{r})$$
$$+N_0^{-1}8\pi a\rho_1 i\,\mathrm{Im}\int d\mathbf{r}K(\mathbf{r},\mathbf{r})\Phi^*(\mathbf{r})^2$$
$$+N_0^{-1}\int d\mathbf{r}[\nabla^2W(\mathbf{r}',\mathbf{r})]_{\mathbf{r}'=\mathbf{r}}. \quad (7.18)$$

8. SOME SIMPLE PROPERTIES OF THE EQUATIONS OF MOTION IN SECOND-ORDER APPROXIMATION

Since the equations of motion (7.13) and (7.14) are rather complicated, only a few simple statements can be made about them. Equation (7.14), being an improvement over (2.21), may be expected to be accurate to the order $(\rho_0 a^3)^{\frac{1}{2}}$ compared with the leading term. On the other hand, certainly only the leading terms in (7.13) are meaningful. Therefore, in general, the equations of motion may be treated in the following manner:

(i) Obtain a first-order approximation to Φ by solving (2.21).

(ii) Use this first-order approximation in (7.13) together with the simplifications

$$\rho_1\rightarrow\rho_0 \quad (8.1)$$

and

$$N_{0t}/N_0\rightarrow 0, \quad (8.2)$$

and solve the resulting simplified equation.

(iii) Use this solution in (7.14) to obtain a second-order approximation to Φ.

The replacement (8.1) is accurate only when

$$N-N_0\ll N, \quad (8.3)$$

and this replacement is not mandatory. However, except for some rather simple cases, it seems difficult to discuss the validity of (7.13) and (7.14) without (8.3).

It is an interesting exercise to work out the case of the ground state with this procedure. If E is the ground state energy per particle and periodic boundary conditions are used, then Φ and K_0 may be written in the form

$$\Phi(\mathbf{r})=e^{-iEt}$$

and

$$K_0(\mathbf{r}',\mathbf{r})=e^{-2iEt}\mathcal{K}_0(\mathbf{r}',\mathbf{r}). \quad (8.4)$$

In carrying out step (ii), it is found that the partial differential equation may be solved by a separation of variables. When L^2/π^2 is an integer, the corresponding homogeneous equation may possess nontrivial solutions; however, since an infinitesimal change in L can make these solutions disappear, they may be considered to be meaningless. When they are omitted, the solution is found to agree with that of Appendix B. It is seen from (B13) that $K(\mathbf{r},\mathbf{r})$ does not exist. Since this divergence is precisely the type encountered by Lee, Huang, and Yang,[3] their procedure of assigning a meaning to $K(\mathbf{r},\mathbf{r})$ may be used before carrying out step (iii). More complicated types of divergence are never encountered in this approximation. It should be noted that the formation as given in Sec. 6 depends critically on the fact that H is Hermitian, and consequently the artifice[10] introduced to deal with the ground state energy is not convenient here.

Consider next the case of a rigid boundary. Here the partial differential equation encountered in step (ii) cannot be solved explicitly. However, some qualitative notion about the solution may be obtained simply by using (8.4) instead. Since the boundary condition on $K_0(\mathbf{r},\mathbf{r}')$ is

$$K_0(\mathbf{r},\mathbf{r}')=0 \quad (8.5)$$

when either $\mathbf{r}$ or $\mathbf{r}'$ is on the boundary S, the solution in this case is

$$\begin{aligned}K_0(x,y,z;\,x',y',z')&=e^{-2iEt}[\mathcal{K}_0(x,y,z;\,x',y',z')-\mathcal{K}_0(x,y,z;\,-x',y',z')\\&\quad-\mathcal{K}_0(x,y,z;\,x',\,-y',z')-\mathcal{K}_0(x,y,z;\,x',y',\,-z')\\&\quad+\mathcal{K}_0(x,y,z;\,x',\,-y',\,-z')+\mathcal{K}_0(x,y,z;\,-x',y',\,-z')\\&\quad+\mathcal{K}_0(x,y,z;\,-x',\,-y',z')\\&\quad-\mathcal{K}_0(x,y,z;\,-x',\,-y',\,-z')]. \quad (8.6)\end{aligned}$$

Since the range of $\mathcal{K}_0$ is of the order of magnitude of the correlation length as defined by (3.21), it is seen that the rigid boundary only has an effect of several correlation lengths, as is the case in the first-order approximation.

The local number density and momentum may be defined by

$$\rho(\mathbf{r})=\langle\Psi|\psi^*(\mathbf{r})\psi(\mathbf{r})|\Psi\rangle, \quad (8.7)$$

and

$$\mathbf{p}(\mathbf{r})=\langle\Psi|\psi^*(\mathbf{r})(1/i)\nabla\psi(\mathbf{r})|\Psi\rangle, \quad (8.8)$$

respectively, while the local velocity is

$$\mathbf{v}(\mathbf{r})=2\mathbf{p}(\mathbf{r})/\rho(\mathbf{r}). \quad (8.9)$$

Note that in (8.8) the gradient operator should operate symmetrically to the right and to the left. Application of rule A to (8.7) and (8.8) gives

$$\rho(\mathbf{r})=\rho_1|\Phi(\mathbf{r})|^2+W(\mathbf{r},\mathbf{r}), \quad (8.10)$$

and

$$\mathbf{p}(\mathbf{r})=\frac{1}{2i}\{\rho_1[\Phi^*(\mathbf{r})\nabla\Phi(\mathbf{r})-\Phi(\mathbf{r})\nabla\Phi^*(\mathbf{r})]$$
$$+[(\nabla-\nabla')W(\mathbf{r}',\mathbf{r})]_{\mathbf{r}'=\mathbf{r}}\}. \quad (8.11)$$

The equation of continuity follows from (7.14) and (7.13) with (8.2). Without any further approximation, it may be verified that

$$\begin{aligned}iW_t(\mathbf{r}',\mathbf{r})&=[-\nabla^2+\nabla'^2+16\pi a\rho_1|\Phi(\mathbf{r})|^2\\&\quad-16\pi a\rho_1|\Phi(\mathbf{r}')|^2]W(\mathbf{r}',\mathbf{r})\\&\quad+8\pi a\rho_1K^*(\mathbf{r}',\mathbf{r})\Phi(\mathbf{r})^2\\&\quad-8\pi a\rho_1K(\mathbf{r}',\ )\end{aligned}$$

and hence

$$\rho_t(\mathbf{r})+2\nabla\cdot\mathbf{p}(\mathbf{r})=0. \tag{8.13}$$

On the other hand, $\mathbf{p}_t(\mathbf{r})$ involves a term of the form

$$\nabla\cdot[(\nabla-\nabla')(\nabla-\nabla')W(\mathbf{r}',\mathbf{r})]_{\mathbf{r}'=\mathbf{r}}, \tag{8.14}$$

which is not expressible in terms of $\rho(\mathbf{r})$ and $\mathbf{v}(\mathbf{r})$. Thus, it is not possible in the second-order approximation to write down an equation of motion of the type of Euler's equation or Navier-Stokes equation.

The vorticity $\nabla\times\mathbf{v}(\mathbf{r})$ involves combinations of the form

$$[(\nabla\times\nabla'-\nabla'\times\nabla)W(\mathbf{r}',\mathbf{r})]_{\mathbf{r}=\mathbf{r}}, \tag{8.15}$$

which does not vanish in general. Therefore, in the second-order approximation, the flow is in general not strictly irrotational.

Finally, the equations of motion are invariant under a Galilean transformation. The rules of the transformation under

$$\mathbf{v}(\mathbf{r})\rightarrow\mathbf{v}(\mathbf{r})+\mathbf{v}_0 \tag{8.16}$$

are

$$\Phi(\mathbf{r})\rightarrow\Phi(\mathbf{r})\exp(i\tfrac{1}{2}\mathbf{v}_0\cdot\mathbf{r}) \tag{8.17}$$

and

$$W(\mathbf{r}',\mathbf{r})\rightarrow W(\mathbf{r}',\mathbf{r})\exp[i\tfrac{1}{2}\mathbf{v}_0\cdot(\mathbf{r}-\mathbf{r}')]. \tag{8.18}$$

9. DISCUSSION

The entire paper is based on specific assumptions about the form of the Schrödinger wave function. These assumptions come from generalizing the one known form of the wave function in the case of the ground state. Accordingly, there is no rigorous proof that the assumptions (2.17) and (6.1) are even approximately valid. The best hope is to justify them *a posteriori* by studying the consequences of these assumptions. This is done to a certain extent in Secs. 4 and 5. The few consequences of the equation of motion in the first-order approximations are not in contradiction with the existing knowledge of nonequilibrium phenomena for a Bose system of hard spheres.

The present theory may also be considered from the point of view that a many-body problem may be described by an infinite system of coupled differential equations of motion for the Green's functions of one particle, two particles, etc. In order to carry out any concrete calculation, this infinite system of equations must be approximated by terminating it in some fashion. This is usually done by approximating the many-particle Green's functions by combinations of those Green's functions involving fewer particles. The assumption on the form of the Schrödinger wave function merely gives a definitive prescription of how this procedure is to be carried out. Since no systematic way to approximate an infinite system of differential equations by a finite one is known, any method of terminating the infinite system is at best heuristic. However, the present procedure does have the advantage of reproducing correctly the lowest stationary state of the Bose system. From this point of view, even in the second-order approximation, only the one-particle Green's function is retained in the finite approximate system of differential equations of motion.

Since the equations of motion (7.13) and (7.14) in the second-order approximation are rather complicated, very little can be done with them. In the following, the compressional wave is to be discussed briefly, taking (7.13) and (7.14) seriously. For this purpose, these equations of motion are linearized by using

$$\Phi(\mathbf{r},t)=e^{-iEt}[1+\epsilon\bar{\Phi}(\mathbf{r},t)], \tag{9.1}$$

$$K_0(\mathbf{r},\mathbf{r}';t)=e^{-2iEt}[\mathcal{K}_0(\mathbf{r},\mathbf{r}')+\epsilon\bar{K}_0(\mathbf{r}',\mathbf{r};t)], \tag{9.2}$$

and retaining only first-order terms. For a given wave number $\mathbf{k}$ for the compressional wave, the step (i) of Sec. 8 gives the following approximation to $\bar{\Phi}(\mathbf{r},t)$:

$$\bar{\Phi}(\mathbf{r},t)=e^{-i(\omega t-\mathbf{k}\cdot\mathbf{r})}-\alpha_k e^{i(\omega t-\mathbf{k}\cdot\mathbf{r})}, \tag{9.3}$$

where ω and k are related by (5.17). When this is used in (7.13), it is seen that $\bar{K}_0$ must have the following invariance property

$$\bar{K}_0(\mathbf{r}+\mathbf{r}_0,\ \mathbf{r}'+\mathbf{r}_0;t)=\bar{K}_0(\mathbf{r},\mathbf{r}';t)\exp(i\mathbf{k}\cdot\mathbf{r}_0). \tag{9.4}$$

This in particular means that N_0 is not changed by the perturbation, i.e., the occupation of the Φ state is not changed by the presence of a compressional wave. This is to be contrasted with the statement that the excitation of a phonon changes the ground-state depletion factor.[11] This difference leads to the result that in the second-order approximation the energy spectrum of a compressional wave is not identical with the phonon spectrum. More precisely, the present calculation indicates that there is a difference between a phonon and a compressional wave in the sense of a periodic variation of Φ when

$$\text{correlation length} \ll \text{wavelength of the compressional wave} \ll \text{thermal wavelength}. \tag{9.5}$$

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APPENDIX A

The derivation of (2.20) from (2.19) is simple if the increment in time is taken to be small compared with $(a\rho_0 N)^{-1}$; however, since the limiting case of infinite volume, and hence infinite N, is not to be excluded, it is

[11] See Sec. 8F of footnote reference 10.

of some interest to see that this assumption about time increment may be replaced by

$$\delta t \ll (a\rho_0)^{-1}. \tag{A1}$$

With this δt, let $[\exp(-iH^{(1)}\delta t)]\Psi(t)$ be computed. For this purpose, calculate first $[\exp(-iH^{(1)}\delta t), a_0^*(t)]$. In general, if

$$[f,g]_1=[f,g] \tag{A2}$$

and

$$[f,g]_n=[f,[f,g]_{n-1}] \tag{A3}$$

for $n>1$, then

$$[e^f,g]=\sum_{n=1}^{\infty}(n!)^{-1}[f,g]_n e^f. \tag{A4}$$

It is straightforward to obtain from (2.13) and (2.14) that

$$[H^{(1)},a_0^*(t)]_{2n}=U^{2n}a_0^*(t), \tag{A5}$$

and

$$[H^{(1)},a_0^*(t)]_{2n+1}=U^{2n}[H_1,a_0^*(t)], \tag{A6}$$

where

$$U^2=\Omega^{-1}\int d\mathbf{r}\,|(-\nabla^2+8\pi a\rho_0|\Phi(\mathbf{r},t)|^2)\Phi(\mathbf{r},t)|^2 - [\tilde{\xi}(t)+8\pi a\rho_0\zeta(t)]^2. \tag{A7}$$

Thus, it follows from (A4) that

$$[\exp(-iH^{(1)}\delta t), a_0^*(t)] = \{a_0^*(t)(\cos U\delta t-1)-iU^{-1}[H^{(1)},a_0^*(t)]\sin U\delta t\} \times\exp(-iH^{(1)}\delta t). \tag{A8}$$

Since U is of the general order of magnitude $a\rho_0$, it follows from (A1) that

$$U\delta t\ll 1. \tag{A9}$$

Consequently, (A8) simplifies to

$$[\exp(-iH^{(1)}\delta t), a_0^*(t)] = -i\delta t[H^{(1)}, a_0^*(t)]\exp(-iH^{(1)}\delta t). \tag{A10}$$

It now follows from (A10) and (2.18) that

$$\exp(-iH^{(1)}\delta t)\Psi(t) = (N!)^{-\frac{1}{2}}\{a_0^*(t)-i\delta t[H^{(1)},a_0^*(t)] - i\delta t[\tilde{\xi}(t)+4\pi a\rho_0\zeta(t)]\}^N|\text{vac}\rangle. \tag{A11}$$

When this is identified with $\Psi(t+\delta t)$, (2.20) results.

APPENDIX B

The case of the ground state of the Bose system may be put in the language of Sec. 6. In the notation of Lee, Huang, and Yang,[3] the ground state is given by

$$\Psi_0=\mathfrak{N}\exp[-\tfrac{1}{2}\sum_{k\neq 0}\alpha_k a_{\mathbf{k}}^* a_{-\mathbf{k}}^*]|\ \rangle, \tag{B1}$$

where

$$\alpha_k=(2y_k)^{-1}[1-(1-4y_k^2)^{\frac{1}{2}}], \tag{B2}$$

$$y_k=4\pi a\rho_0(k^2+8\pi a\rho_0)^{-1}, \tag{B3}$$

$$a_{\mathbf{k}}^*=\Omega^{-\frac{1}{2}}\int d\mathbf{r}\psi^*(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{B4}$$

and $|\ \rangle$ is defined by $a_{\mathbf{k}}|\ \rangle=0$ for all $\mathbf{k}\neq\mathbf{0}$. The state $|\ \rangle$ is to be identified as

$$|\ \rangle=(N!)^{-\frac{1}{2}}a_0^{*N}|\text{vac}\rangle. \tag{B5}$$

Because Ψ_0 is time independent, it should be compared with (6.1) with P in the form [see (8.4)]

$$P=(2N_0)^{-1}\int d\mathbf{r}d\mathbf{r}'\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')\mathcal{K}_0(\mathbf{r},\mathbf{r}')a_0^2. \tag{B6}$$

The result is

$$\mathcal{K}_0(\mathbf{r}',\mathbf{r})=-\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}. \tag{B7}$$

It then follows from analogs of (6.8) and (6.9) that

$$\mathcal{W}_n(\mathbf{r}',\mathbf{r})=\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k^{2n}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \tag{B8}$$

and

$$\mathcal{K}_n(\mathbf{r}',\mathbf{r})=-\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k^{2n+1}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}, \tag{B9}$$

both for $n>1$. From (6.10) and (6.13), it follows that in this case

$$\mathcal{W}(\mathbf{r}',\mathbf{r})=\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k^2(1-\alpha_k^2)^{-1}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}, \tag{B10}$$

and

$$\mathcal{K}(\mathbf{r}',\mathbf{r})=-\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k(1-\alpha_k^2)^{-1}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}. \tag{B11}$$

As $\Omega\to\infty$, these approach, respectively, the limits

$$\mathcal{W}(\mathbf{r}',\mathbf{r})\to(2\pi)^{-3}\int d\mathbf{k}\alpha_k^2(1-\alpha_k^2)^{-1}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}, \tag{B12}$$

and

$$\mathcal{K}(\mathbf{r}',\mathbf{r})\to-(2\pi)^{-3}\int d\mathbf{k}\alpha_k(1-\alpha_k^2)^{-1}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}. \tag{B13}$$

It is important to note that

$$\sum_{n=1}^{\infty}n\mathcal{W}_n(\mathbf{r}',\mathbf{r})=\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k^2(1-\alpha_k^2)^{-2}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}, \tag{B14}$$

and

$$\sum_{n=0}^{\infty}n\mathcal{K}_n(\mathbf{r}',\mathbf{r})=-\Omega^{-1}\sum_{\mathbf{k}=0}\alpha_k^3(1-\alpha_k^2)^{-2}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \tag{B15}$$

both approach finite limiting values as $\Omega\to\infty$, while the limits as $\Omega\to\infty$ of

$$\sum_{n=1}^{\infty}n^2\mathcal{W}_n(\mathbf{r}',\mathbf{r})=\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k^2(1+\alpha_k^2)(1-\alpha_k^2)^{-3}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \tag{B16}$$

and

$$\sum_{n=1}^{\infty}n^2\mathcal{K}_n(\mathbf{r}',\mathbf{r})=-\Omega^{-1}\sum_{\mathbf{k}\neq 0}\alpha_k^3(1+\alpha_k^2)(1-\alpha_k^2)^{-3}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \tag{B17}$$

do not exist.

APPENDIX C

In this Appendix, the formula for $\mathfrak{N}$ [Eq. (6.16)] will be derived, and the rule A of Sec. 6 discussed. It follows directly from (6.2) and (6.6) that

$$\mathfrak{N}^{-2}=\sum_{M=0}^{\infty}\frac{N!}{(N-2M)!M!}(2N_0)^{2M}$$
$$\times\left\langle \text{vac}\left|\left[\int d\mathbf{r}d\mathbf{r}'\psi_1(\mathbf{r})\psi_1(\mathbf{r}')K_0^*(\mathbf{r}',\mathbf{r})\right]^M\right.\right.$$
$$\left.\left.\times\left[\int d\mathbf{r}d\mathbf{r}'\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')K_0(\mathbf{r}',\mathbf{r})\right]^M\right|\text{vac}\right\rangle. \quad \text{(C1)}$$

When an attempt is made to calculate this vacuum expectation value by graphical methods, it is found that the relevant graphs are unions of closed loops. Let m_n be the number of loops consisting of $2n$ links, where each link stands for either K_0 or K_0^*. Because of the conventions (6.4) and (6.5), (C1) can be evaluated by this method as

$$\mathfrak{N}^{-2}=\sum_{M=0}^{\infty}\frac{N!}{(N-2M)!M!}(2N_0)^{-2M}$$
$$\times\sum_{M=\Sigma n m_n}\left[\frac{M!}{\prod_n (n!)^{m_n}}\right]^2\prod_n (m_n!)^{-1}$$
$$\times\prod_n[2^{2n-1}n!(n-1)!\Omega\bar{W}_n]^{m_n}, \quad \text{(C2)}$$

where $\bar{W}_n$ is defined by (6.8), and the factor $2^{2n-1}n!(n-1)!$ comes from the number of different ways of connecting $2n$ points into a loop. Equation (C2) is readily simplified to

$$\mathfrak{N}^{-2}=\sum_{M=0}^{\infty}\frac{N!}{(N-2M)!}N_0^{-2M}$$
$$\times\sum_{M=\Sigma n m_n}\prod_n (m_n!)^{-1}\left(\frac{\Omega\bar{W}_n}{2n}\right)^{m_n}. \quad \text{(C3)}$$

This is to be evaluated for large N.

Define the following two functions of the complex variable z:

$$f_1(z)=\sum_{\{m_n\}} z^{2\Sigma n m_n}\prod_n (m_n!)^{-1}\left(\frac{\Omega\bar{W}_n}{2n}\right)^{m_n}, \quad \text{(C4)}$$

and

$$f_2(z)=\sum_{p=-\infty}^{\infty} z^{-p}\frac{N!}{(N-p)!}N_0^{-p}, \quad \text{(C5)}$$

then

$$\mathfrak{N}^{-2}=\text{coefficient of } z^0 \text{ in } f_1(z)f_2(z). \quad \text{(C6)}$$

Both f_1 and f_2 can be easily evaluated as

$$f_1(z)=\exp\left\{\Omega\sum_n\frac{\bar{W}_n z^{2n}}{2n}\right\}, \quad \text{(C7)}$$

and

$$f_2(z)=(N_0 z)^{-N}N!\exp(N_0 z). \quad \text{(C8)}$$

Thus $z=0$ is a pole of order N for $f_1(z)f_2(z)$. By (C6), it follows from Cauchy's formula that

$$\mathfrak{N}^{-2}=\frac{1}{2\pi i}\oint\frac{f_1(z)f_2(z)dz}{z}, \quad \text{(C9)}$$

where the contour of integration is some circle within which f_1 is analytic. This integral is to be evaluated by the method of steepest descent.

Let W_1 be the operator with matrix elements

$$\langle\mathbf{r}'|W_1|\mathbf{r}\rangle=W_1(\mathbf{r}',\mathbf{r}), \quad \text{(C10)}$$

then

$$\langle\mathbf{r}'|W_1^n|\mathbf{r}\rangle=W_n(\mathbf{r}',\mathbf{r}). \quad \text{(C11)}$$

Furthermore, it follows from (6.7) that W_1 is a non-negative Hermitian operator. Therefore

$$\bar{W}_n=\Omega^{-1}\,\text{Tr}W_1^n\geqslant 0. \quad \text{(C12)}$$

Let λ_0 be the largest eigenvalue of W_1 with degeneracy n_0, then for very large n, $\bar{W}_n$ is given approximately by

$$\bar{W}_n\sim n_0\lambda_0^n. \quad \text{(C13)}$$

It may be concluded from (C12) and (C13) that the function $\sum_n(2n)^{-1}\bar{W}_n z^{2n}$ is analytic in the circle $|z|<\lambda_0^{-1}$, it is increasing and convex along the positive real axis, and it is unbounded as $z\to\lambda_0^{-1}$. Therefore, with (C8), the function $\ln[f_1(z)f_2(z)]$ is strictly convex for $0<z<\lambda_0^{-1}$, and is unbounded near either end. In this range, the equation

$$(d/dz)[f_1(z)f_2(z)]=0 \quad \text{(C14)}$$

has one and only one solution; call it z_0. Furthermore, this is the relevant point of steepest descent since along any circle of constant $|z|$, $|f_1(z)f_2(z)|$ attains its maximum value on the positive real axis. The contour of integration in (C9) is thus chosen to be $|z|=z_0$.

Equation (C14) is more explicitly

$$\Omega\sum_n\bar{W}_n z_0^{2n-1}-N/z_0+N_0=0. \quad \text{(C15)}$$

It is convenient to choose N_0 so that

$$z_0=1. \quad \text{(C16)}$$

The choice is clearly

$$N_0=N-\Omega\bar{W}, \quad \text{(C17)}$$

where

$$\bar{W}=\sum_n\bar{W}_n=\Omega^{-1}\int W(\mathbf{r},\mathbf{r})d\mathbf{r}. \quad \text{(C18)}$$

It will be shown by (C22) that this simple choice implies (6.3). With this choice, (6.16) follows easily from the usual method of steepest descent and Stirling's formula.

If

$$m=O(1), \tag{C19}$$

then

$$\langle\Psi|\,(a_0^*a_0/N_0)^m\,|\Psi\rangle = \mathfrak{N}^2\sum_{M=0}^{\infty}\frac{N!}{(N-2M-m)!}N_0^{-2M-m} \times\sum_{M=\Sigma nm_n}\prod_n(m_n!)^{-1}\left(\frac{\Omega\bar{W}_n}{2n}\right)^{m_n}. \tag{C20}$$

By the method used for $\mathfrak{N}^{-2}$, this is equal to

$$\langle\Psi|\,(a_0^*a_0/N_0)^m\,|\Psi\rangle=\frac{\mathfrak{N}^2}{2\pi i}\oint z^{m-1}f_1(z)f_2(z)dz =1+O(N^{-1}) \tag{C21}$$

as $N\to\infty$. In particular, this shows that

$$N_0=\langle\Psi|\,a_0^*a_0\,|\Psi\rangle+O(1). \tag{C22}$$

The following expectation value may be evaluated by the same procedure:

$$N_0^{-1}\langle\Psi|\,a_0^{*2}\psi_1(\mathbf{r}')\psi_1(\mathbf{r})\,|\Psi\rangle$$

$$=\mathfrak{N}^2N_0^{-1}\sum_{M=0}^{\infty}\frac{N!}{(N-2M-2)!M!(M+1)!}(2N_0)^{-2M-1}\left\langle\mathrm{vac}\left|\left[\int d\mathbf{r}_1d\mathbf{r}_2\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2)K_0^*(\mathbf{r}_1,\mathbf{r}_2)\right]^M\right.\right.$$

$$\left.\left.\times\psi_1(\mathbf{r}')\psi_1(\mathbf{r})\left[\int d\mathbf{r}_1d\mathbf{r}_2\psi_1^*(\mathbf{r}_1)\psi_1^*(\mathbf{r}_2)K_0(\mathbf{r}_1,\mathbf{r}_2)\right]^{M+1}\right|\mathrm{vac}\right\rangle$$

$$=\mathfrak{N}^2\sum_{M=0}^{\infty}\frac{N!}{(N-2M-2)!}N_0^{-2M-2}\sum_m\sum_{\Sigma nm_n=M-m}K_m(\mathbf{r}',\mathbf{r})\prod_n(m_n!)^{-1}\left(\frac{\Omega\bar{W}_n}{2n}\right)^{m_n}$$

$$=\mathfrak{N}^2\frac{1}{2\pi i}\oint K(z^2;\mathbf{r}',\mathbf{r})z^{-1}f_1(z)f_2(z)dz, \tag{C23}$$

where

$$K(z^2;\mathbf{r}',\mathbf{r})=\sum_{n=0}^{\infty}z^{2n+2}K_n(\mathbf{r}',\mathbf{r}). \tag{C24}$$

Since the point of steepest descent is at $z=1$, and from (6.13)

$$K(\mathbf{r}',\mathbf{r})=K(1;\mathbf{r}',\mathbf{r}), \tag{C25}$$

rule A is verified in this special case. In general, rule A can be verified in this manner, although it seems difficult to write down a concise general proof.

It remains to discuss the error involved in using rule A. Consider again the special case (C23). If

$$\lim_{N\to\infty}\frac{\partial^2}{\partial z^2}K(z;\mathbf{r}',\mathbf{r})\Big|_{z=1}$$

exists, then, by the method of steepest descent, the relative error involved in keeping only the leading term is of the order of N^{-1}. This limit is explicitly

$$\lim_{N\to\infty}\sum_{n=0}^{\infty}n(n+1)K_n(\mathbf{r}',\mathbf{r}).$$

By (B17), even in the case of equilibrium, this limit contains a logarithmic divergence. Therefore, the relative error incurred in using rule A in this case is of the order of $N^{-1}\ln N$. This statement is true in general provided that the number of operators in S, $2n+\alpha+\beta$, is of the order of 1 as $N\to\infty$.

APPENDIX D

Rule B of Sec. 6A is not a completely trivial consequence of rule A for the following reason. In connection with the equation of motion, rule B is used, for example, in evaluating the following type of integral:

$$I(S_1,S_2)=\int d\mathbf{r}_1\cdots d\mathbf{r}_{2n}d\mathbf{r}_1'\cdots d\mathbf{r}_{2n'}' \times R(\mathbf{r}_1\cdots\mathbf{r}_{2n})R'(\mathbf{r}_1'\cdots\mathbf{r}_{2n'}') \times[\langle\Psi|\,S_1S_2\,|\Psi\rangle-\langle\Psi|\,S_1\,|\Psi\rangle\langle\Psi|\,S_2\,|\Psi\rangle], \tag{D1}$$

where R and R' are two weight functions which differ appreciably from zero only when all the arguments are close to one another. In this case, the terms obtained by rule B give a contribution to $I(S_1,S_2)$ of the order of N. On the other hand, according to the result of Appendix C, the error term of rule A can contribute something of the order of $N\ln N$. It is necessary to show that this does not occur.

For this purpose, it is sufficient to restrict the attention to those groupings in the S_3 of B(i) that do not mix the $\mathbf{r}$ and the $\mathbf{r}'$ coordinates. These are precisely the groupings excluded in B(iii). Let $I_0(S_1,S_2)$ be the contribution of these groups to $I(S_1,S_2)$. According to

Appendix C, $I_0(S_1,S_2)$ is of the form

$$I_0(S_1,S_2)=\sum\int d\mathbf{r}d\mathbf{r}'R(\mathbf{r})R'(\mathbf{r}')\times\left\{\mathfrak{N}^2\frac{1}{2\pi i}\oint\bar{S}_1(z^2,\mathbf{r})\bar{S}_2(z^2,\mathbf{r}')z^{-1}f_1(z)f_2(z)dz-\mathfrak{N}^4\left[\frac{1}{2\pi i}\oint\bar{S}_1(z^2,\mathbf{r})z^{-1}f_1(z)f_2(z)dz\right]\times\left[\frac{1}{2\pi i}\oint\bar{S}_2(z^2,\mathbf{r}')z^{-1}f_1(z)f_2(z)dz\right]\right\},\quad\text{(D2)}$$

where $\mathbf{r}$ stands symbolically for $\mathbf{r}_1,\cdots\mathbf{r}_{2n}$, and $\mathbf{r}'$ for $\mathbf{r}_1',\cdots\mathbf{r}_{2n'}'$, and the sum is over the types of groupings just mentioned. In (D2), the functions $\bar{S}_1$ and $\bar{S}_2$ are essentially products of the function K of (C24) and a similar one W derived from W_n. To get the leading term of $I_0(S_1,S_2)$, it is sufficient to keep the first and second derivatives of $\bar{S}_1$, and $\bar{S}_2$. Write

$$\bar{S}_1(z^2,\mathbf{r})=\bar{S}_1(1,\mathbf{r})+(z^2-1)\bar{S}_1'(1,\mathbf{r})+\tfrac{1}{2}(z^2-1)^2\bar{S}_1''(1,\mathbf{r}),\quad\text{(D3)}$$

and

$$\bar{S}_2(z^2,\mathbf{r}')=\bar{S}_2(1,\mathbf{r}')+(z^2-1)\bar{S}_2'(1,\mathbf{r}')+\tfrac{1}{2}(z^2-1)^2\bar{S}_2''(1,\mathbf{r}'),\quad\text{(D4)}$$

then the leading term of $I_0(S_1,S_2)$ is

$$I_0(S_1,S_2)=\sum\int d\mathbf{r}d\mathbf{r}'R(\mathbf{r})R'(\mathbf{r}')\left\{\mathfrak{N}^2\frac{1}{2\pi i}\oint[(z^2-1)(\bar{S}_1\bar{S}_2'+\bar{S}_1'\bar{S}_2)+\tfrac{1}{2}(z^2-1)^2(\bar{S}_1\bar{S}_2''+2\bar{S}_1'\bar{S}_2'+\bar{S}_1''\bar{S}_2)]\times z^{-1}f_1(z)f_2(z)dz-\mathfrak{N}^2\left[\frac{1}{2\pi i}\oint[(z^2-1)\bar{S}_1'+\tfrac{1}{2}(z^2-1)^2\bar{S}_1'']z^{-1}f_1(z)f_2(z)dz\right]\bar{S}_2-\mathfrak{N}^2\bar{S}_1\left[\frac{1}{2\pi i}\oint[(z^2-1)\bar{S}_2'+\tfrac{1}{2}(z^2-1)^2\bar{S}_2'']z^{-1}f_1(z)f_2(z)dz\right]\right\}$$

$$=\sum\int d\mathbf{r}d\mathbf{r}'R(\mathbf{r})R'(\mathbf{r}')\bar{S}_1'(1,\mathbf{r})\bar{S}_2'(1,\mathbf{r}')\mathfrak{N}^2\frac{1}{2\pi i}\oint(z^2-1)^2z^{-1}f_1(z)f_2(z)dz.\quad\text{(D5)}$$

Note that $\bar{S}_1''$ and $\bar{S}_2''$ do not appear. Roughly (C7) and (C8) gives

$$\mathfrak{N}^2\frac{1}{2\pi i}\oint(z^2-1)^2z^{-1}f_1(z)f_2(z)dz\sim-4N^{-1}.\quad\text{(D6)}$$

When R and R' are themselves products of $K(\mathbf{r}',\mathbf{r})$ and $W(\mathbf{r}',\mathbf{r})$, the order of magnitufe of $I_0(S_1,S_2)$ may be estimated using the formulas for the ground state. With the results of Appendix B, the estimate is

$$I_0(S_1,S_2)=O[(\rho^{\frac{1}{2}}a^{\frac{3}{2}}\Omega)^2N^{-1}]=O(\rho^2a^3\Omega).\quad\text{(D7)}$$

Similarly, the contribution to $I(S_1,S_2)$ from those terms retained in rule B is of the order of magnitude $\rho^{\frac{1}{2}}a^{\frac{3}{2}}\Omega$. Thus, $I_0(S_1,S_2)$ is smaller by a factor $(\rho a^3)^{\frac{1}{2}}$.

This justifies rule B. It should be emphasized that in connection with (D1) the relative error incurred in using rule B is $(\rho a^3)^{\frac{1}{2}}$, as contrasted with $N^{-1}\ln N$ of rule A.

APPENDIX E

Consider the number-distribution function

$$N(\mathbf{r}',\mathbf{r})=\langle\Psi|\psi^*(\mathbf{r}')\psi(\mathbf{r})|\Psi\rangle.\quad\text{(E1)}$$

Because of (2.6) and (6.1) this can be written as

$$N(\mathbf{r}',\mathbf{r})=\Omega^{-1}\Phi^*(\mathbf{r}')\Phi(\mathbf{r})\langle\Psi|a_0^*a_0|\Psi\rangle+\langle\Psi|\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r})|\Psi\rangle,\quad\text{(E2)}$$

which is easily evaluated by rule A of Sec. 6A:

$$N(\mathbf{r}',\mathbf{r})=\Omega^{-1}N_0\Phi^*(\mathbf{r}')\Phi(\mathbf{r})+W(\mathbf{r}',\mathbf{r}).\quad\text{(E3)}$$

By (C17), (E3) is consistent with the requirement

$$\int d\mathbf{r}N(\mathbf{r},\mathbf{r})=N.\quad\text{(E4)}$$

For an arbitrary one-particle state $\Phi_1(\mathbf{r})$ satisfying

$$\Omega^{-1}\int d\mathbf{r}|\Phi_1(\mathbf{r})|^2=1,\quad\text{(E5)}$$

the corresponding creation and annihilation operators may be defined similar to (2.4):

$$a_1^*=\Omega^{-\frac{1}{2}}\int d\mathbf{r}\psi^*(\mathbf{r})\Phi_1(\mathbf{r})$$

and

$$a_1=\Omega^{-\frac{1}{2}}\int d\mathbf{r}\psi(\mathbf{r})\Phi_1^*(\mathbf{r}).\quad\text{(E6)}$$

The occupation of such a state is

$$n(\Phi_1)=\langle\Psi|a_1^*a_1|\Psi\rangle=\Omega^{-1}\int d\mathbf{r}d\mathbf{r}'\Phi_1(\mathbf{r}')N(\mathbf{r}',\mathbf{r})\Phi_1^*(\mathbf{r}).\quad\text{(E7)}$$

From (E5) and (E7), $n(\Phi_1)$ is stationary if and only if

$$\int d\mathbf{r}'\Phi_1(\mathbf{r}')N(\mathbf{r}',\mathbf{r})=n(\Phi_1)\Phi_1(\mathbf{r}). \tag{E8}$$

Therefore, it follows from (E3) that a possible solution of (E8) is given by

$$\Phi_1(\mathbf{r})=\Phi(\mathbf{r}) \tag{E9}$$

with

$$n(\Phi)=N_0. \tag{E10}$$

Furthermore, since $N(\mathbf{r}',\mathbf{r})$ is a Hermitian kernel, the various solutions of (E8) are orthogonal. Thus any other solution of (E8) satisfies

$$\int d\mathbf{r}'\Phi_1(\mathbf{r}')W(\mathbf{r}',\mathbf{r})=n(\Phi_1)\Phi_1(\mathbf{r}). \tag{E11}$$

Because of (6.12), (E11) may be written as

$$\int d\mathbf{r}'\Phi_1(\mathbf{r}')W_1(\mathbf{r}',\mathbf{r})=[1+n(\Phi_1)]^{-1}n(\Phi_1)\Phi_1(\mathbf{r}). \tag{E12}$$

A consequence of the choice (C17) is that the power series

$$\sum_{n=1}^{\infty} n^{-1}\bar{W}_n z^n$$

is convergent at $z=1$. Thus $1<\lambda_0^{-1}$, or all eigenvalues of the operator W_1 defined by (C10) are less than one. This is consistent with (E12), where $n(\Phi_1)\geqslant 0$.

In particular, for any finite Ω_1 the equation

$$\int d\mathbf{r}'\Phi_1(\mathbf{r}')W_1(\mathbf{r}',\mathbf{r})=\Phi_1(\mathbf{r}) \tag{E13}$$

implies

$$\Phi_1(\mathbf{r})=0. \tag{E14}$$

Since any solution of

$$\int d\mathbf{r}'\Phi_1(\mathbf{r}')K_0^*(\mathbf{r}',\mathbf{r})=\pm\Phi_1^*(\mathbf{r}), \tag{E15}$$

also satisfies (E13), (E15) implies (E14). By Fredholm theory, if Ω is finite and $|f(\mathbf{r})|^2$ is integrable, then the integral equation for $\Phi_1(\mathbf{r})$

$$\int d\mathbf{r}'\Phi_1(\mathbf{r}')W_1(\mathbf{r}',\mathbf{r})=\Phi_1(\mathbf{r})+f(\mathbf{r}) \tag{E16}$$

has one and only one solution. The same is true of the integral equation

$$\int d\mathbf{r}'\Phi_1(\mathbf{r}')K_0^*(\mathbf{r}',\mathbf{r})=\pm\Phi_1^*(\mathbf{r})+f(\mathbf{r}). \tag{E17}$$

This is proved by solving the first iterated integral equation, and then using (E15).

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Dynamics of Nonlinear Stochastic Systems*

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A method for treating nonlinear stochastic systems is described which it is hoped will be useful in both the quantum-mechanical many-body problem and the theory of turbulence. In this method the true problem is replaced by models that lead to closed equations for correlation functions and averaged Green's functions. The model solutions are exact descriptions of possible dynamical systems, and, as a result, they display certain consistency properties. For example, spectral components of Green's functions which must be positive-definite in the true problem automatically are so for the models. The models involve a new stochastic element: Random couplings are introduced among an infinite collection of similar systems, the true problem corresponding to the limit where these couplings vanish. The method is first applied to a linear oscillator with random frequency parameter. The mean impulse-response function of the oscillator is obtained explicitly for two successive models. The results suggest the existence of a sequence of model solutions which converges rapidly to the exact solution of the true problem. Applications then are made to the Schrödinger equation of a particle in a random potential and to Burgers' analog for turbulence dynamics. For both problems, closed model equations are obtained which determine the average Green's function, the amplitude of the mean field, and the covariance of the fluctuating field. The model solutions can be expressed as sums of infinite classes of terms from the formal perturbation expansions of the solutions to the true problems. It is suggested that correspondence to stochastic models may be a useful criterion to help judge the validity of partial summations of perturbation series.

1. INTRODUCTION

THIS paper is intended to introduce a method for treating certain problems where the dynamical equations are nonlinear in stochastic quantities. The quantum-mechanical many-body problem[1,2] and the theory of turbulence[3,4] are two fields of current interest where it is hoped that the method will prove useful. In such problems, there arise from the dynamical equations an infinite hierarchy of coupled equations which relate given ensemble averages to successively more complicated ones. An equivalent statement is that the prediction of a given average over a finite time requires the initial knowledge of an infinite number of averages. This situation, which commonly is called the closure problem, arises even when the nonlinear stochastic terms are linear in the dynamic variables. An example is linear wave propagation in a medium with random refractive index fluctuations.[5] Here the equation for the ensemble-averaged wave amplitude forms the base of an hierarchy involving successively higher cross-moments of the joint distribution of index and amplitude fluctuations.

A formal solution to the dynamical equations of any of the problems mentioned above may be obtained by treating the nonlinear terms as a perturbation and expanding by iteration.[3,6] One may then approximate statistical quantities by either truncating this expansion or summing tractable classes of terms to all orders. Another (and related) approach is to discard the cumulants of the statistical distribution above a certain order. Then all averages are expressible in terms of averages of this order and below, thereby providing a closure of the hierarchy of coupled statistical equations.[2,7]

In the method to be presented here, the true problem is replaced by models that lead, without approximation, to *closed* equations for correlation functions and averaged Green's functions. The model solutions are exact descriptions of possible dynamical systems, and, consequently, they have certain consistency properties which can be lacking in the approximation schemes mentioned. For example, spectral components of Green's functions which must be positive-definite in the true problem automatically are so in the models. A related property is that covariances satisfy certain realizability inequalities.

The models are constructed by introducing dynamical couplings among an infinite collection of similar systems, the true problem corresponding to the limit in which these couplings vanish. The coupling coefficients change randomly from one individual system in the collection to another. Thus they constitute a new stochastic element not present in the true problem. The models are most easily formulated in terms of a collective representation in which the variables are linear combinations of those of all the individual systems.

The closed statistical equations which characterize the models are obtained by averaging over an ensemble of realizations of the collection of coupled systems. When iteration expansions are generated for the averages of basic interest, it is found, using the collective representation, that the random couplings result in the cancellation of large classes of terms of all orders. The

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remaining terms are identical with corresponding ones in the expansion for the true problem (zero couplings). Although still of all orders, they have a sufficiently simple structure so that their sum represents the exact solution of closed integral equations.

The method of stochastic models is introduced in the present paper by application to a linear oscillator whose frequency parameter is Gaussianly distributed over an ensemble. This system has the virtue that it can be solved exactly. Furthermore, it displays great sensitivity to inadequacies in approximation schemes. Neither truncation of the perturbation series nor the cumulant-discard approach yields admissible approximations (Sec. 2). The collective representation and the general model are formulated in Secs. 3 and 4. Explicit solutions for the average impulse-response function of the oscillator then are obtained for two particular models (Secs. 5 and 7). They suggest the existence of a sequence of model solutions which converges rapidly to the exact solution for the true problem. In Sec. 8, model equations are obtained for the mean and covariance of the amplitude of the oscillator when driven by random forces. The generalization to non-Gaussian frequency distributions is described in Sec. 9.

In Sec. 6, approximations for the average response function are examined which represent infinite classes of terms in the perturbation expansion for the true problem, but which do *not* correspond to possible stochastic models. Although they are very plausible in terms of a diagrammatic representation of the perturbation series, these approximations have pathological characteristics. This suggests that correspondence to stochastic models may be a useful criterion to help judge the validity of partial summations of perturbation series in other analogous situations.

In Secs. 10 and 11, stochastic models are formulated for two problems of more physical interest: the Schrödinger equation of a particle in a random potential and Burgers' analog to turbulence dynamics. For both problems, closed integral equations are obtained which determine the average Green's function, the amplitude of the mean field, and the covariance of the fluctuating field. The models for these systems have an intimate formal relation to those for the random oscillator. In fact, the random potential problem is homologous to the oscillator problem, in the sense that the coupling coefficients characterizing corresponding models are identical in the two cases. Many results for the random potential problem can be obtained by inspection from the oscillator results. A comparison of the model equations for the random potential and turbulence problems illustrates the similarities and differences involved when the present method is applied to systems which are, respectively, linear and nonlinear in the dynamic variables.

In a paper to follow, stochastic models are formulated for classical and quantized nonlinear oscillators. Then the many-boson problem with interparticle forces is treated. This problem is homologous to the quantized nonlinear oscillator in the same way as the random potential problem is to the classical random linear oscillator. Particular attention is given to thermal equilibrium. The Einstein-Bose distribution law is derived by requiring equilibrium under arbitrary infinitesimal changes in the coupling among systems in a collection, without assuming a grand canonical or other particular distribution.

2. RANDOM OSCILLATOR

Let the amplitude $q(t)$ of a linear oscillator satisfy

$$dq(t)/dt+ibq(t)=0, \tag{2.1}$$

where b is a real time-independent parameter which is statistically distributed over an infinite ensemble of realizations of the oscillator. We shall be interested in determining the function $G(t)=\langle G_{[\,]}(t)\rangle$, where $\langle\ \rangle$ denotes ensemble average and $G_{[\,]}(t)$ is the response function[8] defined for $-\infty<t<\infty$ by

$$dG_{[\,]}(t)/dt=-ibG_{[\,]}(t),\quad G_{[\,]}(0)=1. \tag{2.2}$$

We have, immediately,

$$G(t)=\langle\exp(-ibt)\rangle=\int_{-\infty}^{\infty}\exp(-ibt)P(b)db,$$

where $P(b)$ is the normalized probability density for b. Hence,

$$\tilde{G}(\omega)=P(\omega), \tag{2.3}$$

where

$$\tilde{G}(\omega)=(2\pi)^{-1}\int_{-\infty}^{\infty}G(t)\exp(i\omega t)dt.$$

Since $P(b)\geq 0$, $\tilde{G}(\omega)$ must satisfy the realizability condition

$$\tilde{G}(\omega)=|\tilde{G}(\omega)|. \tag{2.4}$$

A particular consequence of Eq. (2.4) is

$$|G(t)|\leq G(0)=1, \tag{2.5}$$

which also follows from the fact that $|q(t)|$ is a constant of motion in each realization of the oscillator.

Now suppose that $P(b)$ is not known in closed form, but instead is specified by the infinite set of moments $\langle b\rangle$, $\langle b^2\rangle$, $\langle b^3\rangle$, $\cdots$. Then, by integrating Eq. (2.2) from 0 to t, iterating, and averaging, we may generate the formal solution.

$$G(t)=1+\sum_{n=1}^{\infty}(-i)^n\langle b^n\rangle t^n/n!. \tag{2.6}$$

Equation (2.6) corresponds precisely to the perturbation series for the averaged Green's function in certain statistical field physics problems. Let us explore its validity for the present problem by taking the

[8] The reason for the peculiar bracket notation will become clear in Sec. 3.

example of Gaussian $P(b)$. Then we have

$$\tilde{G}(\omega)=(2\pi\langle b^2\rangle)^{-\frac{1}{2}}\exp(-\tfrac{1}{2}\omega^2/\langle b^2\rangle), \tag{2.7}$$

$$G(t)=\exp(-\tfrac{1}{2}\langle b^2\rangle t^2). \tag{2.8}$$

But let us suppose that we do not know this closed form and instead are given the moment values

$$\langle b^n\rangle=0 \quad (n \text{ odd}), \quad \langle b^{2n}\rangle=(\tfrac{1}{2}\langle b^2\rangle)^n 2n!/n!. \tag{2.9}$$

By Eq. (2.6) we have

$$G(t)=1+\sum_{n=1}^{\infty}(-\tfrac{1}{2}\langle b^2\rangle t^2)^n/n!, \tag{2.10}$$

which, of course, is the power series expansion of Eq. (2.8).

The following observations may be made concerning Eq. (2.10). First, it is absolutely convergent for all t. Second, for $t>2/\langle b^2\rangle^{\frac{1}{2}}$ the convergence rapidly becomes very poor so that very many terms must be taken to obtain a good approximation. Third, if the series is truncated after any finite number of terms, we have $G(t)\to\infty$, $t\to\infty$, in violation of the basic realizability condition (2.5). Thus, at no finite stage of the iteration treatment do we obtain an approximation with uniform validity for all t, and, in particular, at no stage does the spectral density $\tilde{G}(\omega)$ exist.

Let us next apply a second approximation scheme which has been widely used in statistical field physics. From Eq. (2.2) we may obtain the infinite set of coupled equations

$$\begin{aligned}
&dG(t)/dt=-i\langle bG_{[\ ]}(t)\rangle && G(0)=1,\\
&d\langle bG_{[\ ]}(t)\rangle/dt=-i\langle b^2G_{[\ ]}(t)\rangle && \langle bG_{[\ ]}(0)\rangle=0,\\
&d\langle b^2G_{[\ ]}(t)\rangle/dt=-i\langle b^3G_{[\ ]}(t)\rangle && \langle b^2G_{[\ ]}(0)\rangle=\langle b^2\rangle,\\
&\qquad\cdots
\end{aligned} \tag{2.11}$$

We may close off this hierarchy at successively higher stages by taking the zeroth approximation that b and $G_{[\ ]}(t)$ are statistically independent, and then admitting successively higher-order cumulants of the joint distribution (higher "correlations" in the language of statistical field physics). Let us again assume Eq. (2.9). Then the appropriate successive closure approximations are

$$\begin{aligned}
&\langle bG_{[\ ]}(t)\rangle=\langle b\rangle G(t)=0,\\
&\langle b^2G_{[\ ]}(t)\rangle=\langle b^2\rangle G(t),\\
&\langle b^3G_{[\ ]}(t)\rangle=3\langle b^2\rangle\langle bG_{[\ ]}(t)\rangle,\\
&\langle b^4G_{[\ ]}(t)\rangle=6\langle b^2\rangle\langle b^2G_{[\ ]}(t)\rangle-3\langle b^2\rangle^2G(t),\\
&\qquad\cdots
\end{aligned} \tag{2.12}$$

[Note that if $G_{[\ ]}(t)$ were statistically independent of b then all these relations would be exact.] On using these relations in turn to close off Eq. (2.11) at successively higher stages, we obtain

$$\begin{aligned}
&G(t)=1,\\
&G(t)=\cos(b_*t),\\
&G(t)=\tfrac{2}{3}+\tfrac{1}{3}\cos(\sqrt{3}b_*t),\\
&G(t)=\tfrac{1}{6}(3+\sqrt{6})\cos[(3-\sqrt{6})^{\frac{1}{2}}b_*t]\\
&\qquad+\tfrac{1}{6}(3-\sqrt{6})\cos[(3+\sqrt{6})^{\frac{1}{2}}b_*t],\\
&\qquad\cdots,
\end{aligned} \tag{2.13}$$

where $b_*=\langle b^2\rangle^{\frac{1}{2}}$.

Beyond the zeroth stage, which yields identical results in the two cases, the sequence (2.13) is distinctly superior to the approximations obtained by truncating Eq. (2.10). All members of the sequence satisfy Eqs. (2.4) and (2.5). In common with the iteration scheme, the first n even derivatives of $G(t)$ at $t=0$ are correct in the nth approximation. However, there still is no uniform validity in the sense $G(t)\to 0$, $t\to\infty$. None of the moments $\int_0^\infty t^nG(t)dt$ $(n=1, 2, \cdots)$ exist for any approximation in the sequence, whereas they all do for the exact solution. Alternatively, we may note that $\tilde{G}(\omega)$, which is smooth in the exact solution, is a sum of δ functions in any of the cumulant-discard approximations. The convergence to the exact $G(t)$ is still very poor for $t>2/b_*$.

It is clear that the random oscillator exhibits in acute form certain shortcomings of the iteration (perturbation) and cumulant-discard approaches to dynamical equations which are nonlinear in stochastic quantities. Both for this reason and because of its simplicity, we shall use the random oscillator to illustrate the alternative approach which is the subject of this paper. The sensitivity to inadequacies in the method of approximation arises because the solution to the "unperturbed" equation, obtained by replacing the right-hand side of Eq. (2.2) with zero, has a monochromatic spectrum. In this respect, it resembles certain limiting cases of statistical field theory problems which are of current interest and to which our approach will be applicable. Examples are a quantum-mechanical particle in a random potential in the WKBJ limit, turbulence at infinite Reynolds number, and, in a less direct sense, a second-quantized many-boson system at very low temperature.

3. COLLECTIVE REPRESENTATION FOR A SET OF OSCILLATORS

We shall now describe a dynamical representation which is appropriate for formulating the stochastic models promised in Sec. 1. We shall introduce the representation formally and then give a physical interpretation and a comparison with more familiar concepts.

In Sec. 2 we treated an ensemble of realizations of a single oscillator. Now let us consider a collection of M oscillators ($M=2S+1$, $S=$positive integer) whose frequencies are identically and independently distributed over an ensemble of realizations of the collection. We

shall be interested in the limit $M \to \infty$, so that in reality we are introducing a kind of two-dimensional distribution. In place of the frequencies and amplitudes of the M individual oscillators, let us adopt the collective parameters and coordinates

$$\begin{aligned} b_\alpha &= M^{-\frac{1}{2}} \textstyle\sum_n \exp(i2\pi\alpha n/M) b_{[n]}, \\ q_\alpha(t) &= M^{-\frac{1}{2}} \textstyle\sum_n \exp(i2\pi\alpha n/M) q_{[n]}(t), \\ (\alpha &= 0, \pm 1, \cdots, \pm S) \quad (n = 1, 2, \cdots, M), \end{aligned} \tag{3.1}$$

where $b_{[n]}$ and $q_{[n]}(t)$ are the frequency and amplitude of the nth oscillator.[9] The identities

$$\begin{aligned} M^{-1} \textstyle\sum_\alpha \exp[i2\pi\alpha(n-m)/M] &= \delta_{n,m}, \\ M^{-1} \textstyle\sum_n \exp[i2\pi n(\alpha-\beta)/M] &= \delta_{\alpha,\beta} \end{aligned} \tag{3.2}$$

yield

$$\begin{aligned} b_{[n]} &= M^{-\frac{1}{2}} \textstyle\sum_\alpha \exp(-i2\pi\alpha n/M) b_\alpha, \\ q_{[n]}(t) &= M^{-\frac{1}{2}} \textstyle\sum_\alpha \exp(-i2\pi\alpha n/M) q_\alpha(t). \end{aligned} \tag{3.3}$$

Let us adopt hereafter the cyclic convention $\alpha \pm M \equiv \alpha$, which clearly is consistent with Eqs. (3.1) and (3.3).

From Eqs. (3.1) and (3.2) we easily find

$$\begin{aligned} b_{-\alpha} &= b_\alpha^*, \quad \textstyle\sum_\alpha b_\alpha b_{-\alpha} = \sum_n b_{[n]}^2, \\ \textstyle\sum_\alpha q_\alpha(t) q_\alpha^*(t') &= \textstyle\sum_n q_{[n]}(t) q_{[n]}^*(t'), \end{aligned} \tag{3.4}$$

where we have used $b_{[n]} = b_{[n]}^*$. From the equations of motion

$$dq_{[n]}(t)/dt + ib_{[n]} q_{[n]}(t) = 0, \tag{3.5}$$

we find

$$dq_\alpha(t)/dt = -iM^{-\frac{1}{2}} \textstyle\sum_\beta b_\beta q_{\alpha-\beta}(t), \tag{3.6}$$

where $\alpha-\beta$ is to be interpreted according to the cyclic convention. This shows that the new coordinates, in contrast to the old, are dynamically coupled. By Eq. (3.4), $\sum_\alpha q_\alpha(t) q_\alpha^*(t)$ is a constant of motion. Let $G_{[n,m]}(t)$ denote the solution of Eq. (3.5) with $q_{[r]}(0) = \delta_{r,m}$ (all r) and let $G_{\alpha,\gamma}(t)$ denote the solution of Eq. (3.6) with $q_\mu(0) = \delta_{\mu,\gamma}$ (all μ). Since the individual oscillators are uncoupled, we have $G_{[n,m]}(t) = \delta_{n,m} G_{[n,n]}(t)$. Hence, by Eqs. (31.) and (3.3), and the linearity of the equations of motion,

$$G_{\alpha,\gamma}(t) = M^{-1} \textstyle\sum_n \exp[i2\pi(\alpha-\gamma)n/M] G_{[n,n]}(t). \tag{3.7}$$

The functions $G_{\alpha,\gamma}(t)$ constitute the response matrix of the collection of oscillators in the new representation, and the $G_{[n,m]}(t)$ play this role in the old representation.

The statistical properties of the b_α are easily found from the assumption that the $b_{[n]}$ are identically and independently distributed. By Eqs. (3.1) and (3.2), we have immediately

$$\langle b_\alpha b_\beta \cdots b_\mu \rangle = 0 \quad (\alpha+\beta+\cdots+\mu \neq 0). \tag{3.8}$$

For Gaussian $b_{[n]}$ all odd-order moments vanish, and we have

$$\begin{aligned} \langle b_{[n]} b_{[m]} \rangle &= \delta_{n,m} \langle b^2 \rangle, \\ \langle b_{[n]} b_{[m]} b_{[r]} b_{[s]} \rangle &= (\delta_{n,m}\delta_{r,s} + \delta_{n,r}\delta_{m,s} + \delta_{n,s}\delta_{m,r}) \langle b^2 \rangle^2, \\ &\cdots, \end{aligned} \tag{3.9}$$

where $\langle b^2 \rangle = \langle b_{[n]}^2 \rangle$, which is the same for all n. Then, by Eq. (3.1),

$$\begin{aligned} \langle b_\alpha \cdots b_\mu \rangle &= 0 \quad \text{(odd number of factors)}, \\ \langle b_\alpha b_\beta \rangle &= \delta_{\alpha+\beta} \langle b^2 \rangle \quad (\delta_{\alpha+\beta} \equiv \delta_{0,\alpha+\beta}), \\ \langle b_\alpha b_\beta b_\gamma b_\epsilon \rangle &= (\delta_{\alpha+\beta}\delta_{\gamma+\epsilon} + \delta_{\alpha+\gamma}\delta_{\beta+\epsilon} + \delta_{\alpha+\epsilon}\delta_{\beta+\gamma}) \langle b^2 \rangle^2, \\ &\cdots. \end{aligned} \tag{3.10}$$

For any univariate $b_{[n]}$ distribution we find from Eq. (3.7),

$$\begin{aligned} \langle G_{\alpha,\beta}(t) \rangle &= \delta_{\alpha,\beta} G(t), \\ \langle b_\beta G_{\gamma,\alpha}(t) \rangle &= \delta_{\alpha,\beta+\gamma} M^{-\frac{1}{2}} \langle b G_{[\,]}(t) \rangle, \\ \langle G_{\alpha,\gamma}(t) G_{\gamma,\alpha}^*(t) \rangle &= \delta_{\alpha,\gamma} |G(t)|^2 + M^{-1} [\langle |G_{[\,]}(t)|^2 \rangle - |G(t)|^2]. \end{aligned} \tag{3.11}$$

Here $G_{[\,]}(t)$ denotes $G_{[n,n]}(t)$, which is the same for all n, and $G(t) = \langle G_{[\,]}(t) \rangle$, as in Sec. 2. In the limit $M \to \infty$, with which we are concerned, Eq. (3.11) gives

$$\begin{aligned} &\langle G_{\alpha,\alpha}(t) \rangle = G(t), \quad \langle |G_{\alpha,\alpha}(t) - G(t)|^2 \rangle = O(M^{-1}), \\ &\langle G_{\alpha,\gamma}(t) G_{\gamma,\alpha}^*(t) \rangle = O(M^{-1}) \quad (\alpha \neq \gamma), \\ &\langle b_\gamma G_{\alpha-\gamma,\alpha}(t) \rangle = O(M^{-\frac{1}{2}}). \end{aligned} \tag{3.12}$$

These relations show that the variance of

$$G_{\alpha,\alpha}(t) = M^{-1} \textstyle\sum_n G_{[n,n]}(t)$$

vanishes in the limit. That is, $G_{\alpha,\alpha}(t)$ is statistically *sharp*. They further imply that the effective dynamical coupling between any given pair of degrees of freedom q_α and q_γ is infinitely weak in the limit. Equations (3.12) were obtained without explicit reference to Eq. (3.6), but their dynamical implications may also be inferred from the latter. The direct dynamical coupling of q_α to any q_γ arises from only one of the M terms, each $O(M^{-\frac{1}{2}})$, on the right-hand side of Eq. (3.6). Equations (3.12) show that the effective coupling is still $O(M^{-\frac{1}{2}})$ when the indirect interaction of q_α and q_γ through all the other degrees of freedom is included. The absence of fluctuations in $G_{\alpha,\alpha}(t)$ in the limit is consistent with the fact that this function is determined by the simultaneous interaction of q_α with an infinite number of other degrees of freedom; q_α exhibits negligible self-coupling, in contrast to $q_{[n]}$.

It is apparent, both from Eq. (3.1) and the convolution structure of Eq. (3.6), that the q_α have a close formal relation to Fourier coefficients. The physical significance of the new representation is best brought out, in fact, by a comparison with analysis into wave-number or frequency components. Let $\psi(x,t)$ be a scalar field, associated with an extended (one-dimensional) dynamical system, which is described by an

[9] Throughout this paper, quantities referring to individual systems will be labeled with square-bracketed Latin indices and collective quantities will be labeled with unbracketed Greek indices.

ensemble statistically invariant under translation (e.g., $\langle\psi(x,t)\psi(x',t)\rangle=\langle\psi(x+y,t)\psi(x'+y,t)\rangle$ for all y). The natural coordinates for describing the field then are wavenumber components, which change only by a phase factor under translation. Suppose, instead, the ensemble were invariant under time displacement. Then the natural coordinates would be frequency components.

Physical systems usually are neither statistically homogeneous nor stationary. However, if we form a collection of identically distributed individual systems, then obviously (and, it will appear at first sight, trivially) there is statistical invariance under permutation within the collection. The new representation is natural in the presence of this invariance in the same way that a wavenumber representation is natural when there is translational invariance. Actually, the permutation invariance is much broader than called for by strict analogy to translational invariance. Consequently, all the q_α ($\alpha\neq 0$) have identical statistical properties,[10] while, in general, the statistical properties of wavenumber components vary with wave number.

To examine the analogy further, let us take

$$\psi_k(t)=L^{-1}\int_{-L/2}^{L/2}\psi(x,t)\exp(-ikx)dx \qquad (k=2\pi\alpha/L,\ \alpha=0,\pm1,\cdots),$$

where we adopt the customary device of making the field cyclic with a period L which is as large as we wish compared to any relevant correlation length. Let us divide L into very many segments, each still very large compared to any correlation length. Then each segment contains a subsystem which has only a negligible statistical dependence on its neighbors. Furthermore, it is plausible to suppose that (over times which are not too large) each subsystem has only a negligible dynamical interaction with its neighbors. Then we validly may regard the set of subsystems as analogous to the collection of *perfectly* independent systems used above in defining the q_α. Considered in this way, the ψ_k and the q_α (for large M) play essentially similar roles. Both are linear combinations of the physical coordinates of a very large number of effectively independent systems.[11]

4. FORMULATION OF MODEL PROBLEMS

Consider, instead of Eq. (3.6), the more general equations

$$dq_\alpha(t)/dt=-iM^{-\frac{1}{2}}\textstyle\sum_\beta \phi_{\alpha,\beta,\alpha-\beta}b_\beta q_{\alpha-\beta}(t), \qquad (4.1)$$

where $\phi_{\alpha,\beta,\alpha-\beta}$ is independent of t and the same for every realization in the ensemble. We shall be interested in stochastic assignments of $\phi_{\alpha,\beta,\alpha-\beta}$ in the sense that this quantity will exhibit random changes in value as α and β are changed. By Eqs. (3.3) and (3.2), Eq. (4.1) implies

$$dq_{[n]}(t)/dt=-i\textstyle\sum_{r,s}A_{[n,r,s]}b_{[r]}q_{[s]}(t), \qquad (4.2)$$

where

$$A_{[n,r,s]}=M^{-2}\textstyle\sum_{\beta,\gamma}\exp\{i2\pi[\beta(r-n)+\gamma(s-n)]/M\}\phi_{\beta+\gamma,\beta,\gamma}. \qquad (4.3)$$

Thus, the individual oscillators in the collection now are dynamically coupled. When $\phi_{\alpha,\beta,\alpha-\beta}=1$ for all α and β, then $A_{[n,r,s]}=\delta_{r,n}\delta_{s,n}$ so that we recover the original collection of uncoupled oscillators. The quantities $q_{[n]}(t)q_{[n]}{}^*(t)$ are no longer constants of motion in the general case. However, we shall require

$$\phi_{\alpha,\beta,\alpha-\beta}=\phi_{\alpha-\beta,-\beta,\alpha}{}^*. \qquad (4.4)$$

Then, since $b_{-\beta}=b_\beta{}^*$, we find

$$d(\textstyle\sum_n q_{[n]}q_{[n]}{}^*)/dt=d(\sum_\alpha q_\alpha q_\alpha{}^*)/dt=0. \qquad (4.5)$$

The response matrix corresponding to Eq. (4.1) satisfies

$$dG_{\alpha,\gamma}(t)/dt=-iM^{-\frac{1}{2}}\textstyle\sum_\beta\phi_{\alpha,\beta,\alpha-\beta}b_\beta G_{\alpha-\beta,\gamma}(t), \quad G_{\alpha,\gamma}(0)=\delta_{\alpha,\gamma}. \qquad (4.6)$$

Suppose that we carry out an iteration expansion of Eq. (4.6). The coefficient of t^n in the resulting power series for $G_{\alpha,\gamma}(t)$ is a sum over products of n factors ϕ and n factors b. It is clear, from the initial condition and the way the indices combine, that in each product the sum of the indices of the b factors must be $\alpha-\gamma$. Hence, by Eq. (3.8),

$$\langle G_{\alpha,\gamma}(t)\rangle=0 \quad (\alpha\neq\gamma). \qquad (4.7)$$

By Eqs. (3.1), (3.3), and (4.7), we have

$$\langle G_{[n,m]}(t)\rangle=M^{-1}\textstyle\sum_\alpha\exp[-i2\pi(n-m)\alpha/M]\langle G_{\alpha,\alpha}(t)\rangle. \qquad (4.8)$$

Therefore, if $\langle G_{\alpha,\alpha}(t)\rangle$ is independent of α, we have, by Eq. (3.2),

$$\langle G_{[n,m]}(t)\rangle=\delta_{n,m}G(t), \quad G(t)=\langle G_{\alpha,\alpha}(t)\rangle, \qquad (4.9)$$

where $G(t)$ has now the same meaning as in Sec. 3. We shall be concerned only with ϕ assignments which yield Eq. (4.9), and, presently, we shall exhibit certain of their properties.

We wish now to develop an expression for $d\langle G_{\alpha,\alpha}(t)\rangle/dt$ by expanding the right-hand side of Eq. (4.6), with $\gamma=\alpha$. By writing

$$H_{\alpha-\beta,\beta,\alpha}(t)=-iM^{-\frac{1}{2}}\phi_{\alpha,\beta,\alpha-\beta}b_\beta G_{\alpha-\beta,\alpha}(t), \qquad (4.10)$$

we may develop $\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle$ in powers of t by using the iteration expansion for $G_{\alpha-\beta,\alpha}(t)$. The coefficient of t^{r-1} in the resulting series is a sum, over the indices of all b factors except b_β, of products of r factors b and r

[10] The special role played by $\alpha=0$ will become clear in Sec. 8.

[11] It is of interest to indicate how the q_α might be measured, in principle. Let a device sample each oscillator in the collection in turn, at time intervals τ, proceeding in order of increasing n and returning from the Mth oscillator to the first to repeat the cycle continuously. At each sampling instant let the device produce a sharp pulse, of strength proportional to $q_{[n]}(t)$. If τ is small enough that many cycles are completed before the $q_{[n]}$ change appreciably, the spectrum of the pulse train will approximate a line spectrum with frequencies $\alpha/M\tau$ and amplitudes proportional to the $q_\alpha(t)$.

factors ϕ [including the factors b_β and $\phi_{\alpha,\beta,\alpha-\beta}$ which appear explicitly in Eq. (4.10)]. Let us take Gaussian $b_{[n]}$. (We shall return to the general case in Sec. 9.) Then, by Eqs. (3.8) and (3.10), only the odd powers of t survive and in the coefficients of these the indices of the b factors must be equal and opposite in pairs. In this way we find

$$\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle = M^{-1}\sum_{n=1}^{\infty}\sum_{p}(-1)^n C_{2n;p}(\alpha,\beta,\alpha-\beta) \times\langle b^2\rangle^n t^{2n-1}/(2n-1)!, \quad (4.11)$$

where $M^{n-1}C_{2n;p}(\alpha,\beta,\alpha-\beta)$ is a sum of products of $2n$ factors ϕ and the index p ($p=1, 2, \cdots, 2n!/2^n n!$) labels (in an arbitrary order) the contributions which arise from all the possible pairings of the b factors.

The $C_{2n;p}(\alpha,\beta,\alpha-\beta)$ through $n=2$ are

$$\begin{aligned}
C_{2;1}(\ ) &= \phi_{\alpha,\beta,\alpha-\beta}\phi_{\alpha-\beta,-\beta,\alpha},\\
C_{4;1}(\ ) &= M^{-1}\textstyle\sum_\gamma \phi_{\alpha,\beta,\alpha-\beta}\phi_{\alpha-\beta,-\beta,\alpha}\phi_{\alpha,\gamma,\alpha-\gamma}\phi_{\alpha-\gamma,-\gamma,\alpha},\\
C_{4;2}(\ ) &= M^{-1}\textstyle\sum_\gamma \phi_{\alpha,\beta,\alpha-\beta}\phi_{\alpha-\beta,\gamma,\alpha-\beta-\gamma}\\
&\quad\times\phi_{\alpha-\beta-\gamma,-\gamma,\alpha-\beta}\phi_{\alpha-\beta,-\beta,\alpha},\\
C_{4;3}(\ ) &= M^{-1}\textstyle\sum_\gamma \phi_{\alpha,\beta,\alpha-\beta}\phi_{\alpha-\beta,\gamma,\alpha-\beta-\gamma}\\
&\quad\times\phi_{\alpha-\beta-\gamma,-\beta,\alpha-\gamma}\phi_{\alpha-\gamma,-\gamma,\alpha}.
\end{aligned} \quad (4.12)$$

The ϕ factors in Eqs. (4.12) other than $\phi_{\alpha,\beta,\alpha-\beta}$ are written from the right in the order in which they arise in the iteration process. (The values of p are assigned arbitrarily.)

Each $C_{2n;p}(\alpha,\beta,\alpha-\beta)$ is closed in the sense that the initial index on any factor equals the final index on the factor to its immediate left [when ordered as in Eqs. (4.12)] while the middle indices are equal and opposite in pairs. This permits a systematic diagrammatic representation of the $C_{2n;p}(\alpha,\beta,\alpha-\beta)$ and therefore of Eq. (4.11). With each $\phi_{\mu,\lambda,\sigma}$ or $\phi_{\mu,\lambda,\sigma}{}^*$ let us associate a vertex as shown in Fig. 1(a) or 1(b), respectively. The $C_{2n;p}(\alpha,\beta,\alpha-\beta)$ then may be obtained by the following rules:

Connect $2n$ points by $2n$ solid line segments to form a single closed loop; then connect all the points in pairs by n dashed line segments to form a closed diagram of $2n$ vertices. Equip all the solid line segments with arrows pointing in the same sense. Choose one vertex, equip its dashed line segment with an ingoing arrow, and label its three line segments to correspond to $\phi_{\alpha,\beta,\alpha-\beta}$ in the sense of Fig. 1(a). Call this the fixed vertex and identify it by circling. Label the remaining dashed line segments $\gamma, \epsilon, \cdots$ in any order and equip them with arrows (whose direction does not matter).[12] Complete the labeling of the solid line segments so that the sum of the indices labeling the ingoing lines equals the sum of those labeling the outgoing lines at every vertex. Now write the product of the ϕ factors associated with all the vertices according to Fig. 1(a), or according to Fig. 1(b) and Eq. (4.4). For each n there are $2n!/2^n n!$ distinct diagrams of this type, corresponding to the $2n!/2^n n!$ ways of connecting the vertices by dashed lines after one is chosen as the fixed vertex. Each diagram

FIG. 1. Vertices representing $\phi_{\mu,\lambda,\sigma}$ and $\phi_{\mu,\lambda,\sigma}{}^*$ for the random oscillator.

corresponds to one $C_{2n;p}(\alpha,\beta,\alpha-\beta)$ (according to an arbitrary rule for assigning the values of p) and the latter is equal to M^{1-n} times the sum over $\gamma, \epsilon, \cdots$ of the associated ϕ product.

The diagrams associated with Eqs. (4.12) are shown in Fig. 2.

It is clear from Eq. (4.11) that $\langle G_{\alpha,\alpha}(t)\rangle$ will be independent of α, and therefore Eq. (4.9) will hold, if

$$M^{-1}\textstyle\sum_\beta C_{2n;p}(\alpha,\beta,\alpha-\beta) = C_{2n;p}, \quad (4.13)$$

where $C_{2n;p}$ is independent of α. In this case,

$$G(t) = 1+\sum_{n=1}^{\infty}\sum_{p}(-1)^n C_{2n;p}\langle b^2\rangle^n t^{2n}/2n!. \quad (4.14)$$

We shall be concerned hereafter only with ϕ assignments such that Eq. (4.13) is satisfied when $M\to\infty$. The $C_{2n;p}$ may be interpreted as moments of the distribution of the quantity $\phi_{\mu,\lambda,\mu-\lambda}$ over the set of index values μ and λ.

Let us associate with $C_{2n;p}$ the diagram for $C_{2n;p}(\alpha,\beta,\alpha-\beta)$, but with index labels and dashed line arrows (which are now superfluous) omitted. By Eq. (4.13), we have $C_{2n;p}=M^{-2}\sum_{\alpha,\beta}C_{2n;p}(\alpha,\beta,\alpha-\beta)$. Recalling the cyclic convention $\mu\equiv\mu\pm M$ (any μ), we see that the summation in this expression is equivalent to one over all M values of all the indices labeling lines in the diagram, subject only to the sum condition at each vertex. Consequently, the expression is independent of which is the fixed vertex; its value depends only on the order and topology of the diagram.

It is important to point out that Eq. (3.12) is valid for general ϕ's satisfying Eq. (4.13). In particular, $G_{\alpha,\alpha}(t)$ is statistically sharp ($M\to\infty$). In the original case (all ϕ's unity) this was so because q_α interacted simultaneously with all the other degrees of freedom, and negligibly with itself. These properties clearly characterize the general case also, provided the ϕ's are bounded as $M\to\infty$. The validity of Eq. (3.12) in the general case is easily demonstrated[13] for any power of t

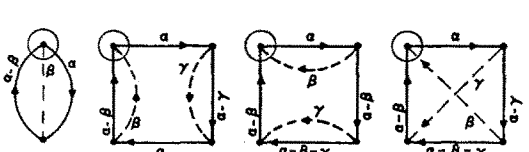

FIG. 2. Diagrams for $C_{2;1}(\ )$, $C_{4;1}(\ )$, $C_{4;2}(\ )$, and $C_{4;3}(\ )$.

[12] Reversal of the direction of the arrow on a dashed line labeled λ corresponds to the trivial notation change $\lambda\to-\lambda$ for the summed index λ in the associated $C_{2n;p}(\alpha,\beta,\alpha-\beta)$.

[13] See Appendix A. (a) Our "irreducible" diagrams are "proper" diagrams in the terminology of quantum field theory.

in the iteration expansion of the left sides of the equations, if one uses Eq. (3.10) and the fact that the ϕ's are the same for all realizations. We shall use the abbreviations C and $C(\ )$ to denote $C_{2n;p}$ and $C_{2n;p}(\alpha,\beta,\alpha-\beta)$, respectively, when it is not desired to specify particular subscripts and arguments.

Let us define a reducible C as one which may be factored into two or more C's of lower order, and an irreducible C as one which may not. Let us define a reducible $C(\ )$ as one which may be factored into the product of a lower-order $C(\ )$ with one or more C's, and an irreducible $C(\ )$ as one which may not. It follows that each reducible C is a product of irreducible C's and each reducible $C(\ )$ is a product of an irreducible $C(\ )$ with irreducible C's. It is easy to see from our rules that reducible $C(\ )$'s and C's (and only they) are associated with diagrams in which there is a part, or parts, connected to the rest of the diagram by only solid lines.[13a] Thus, $C_{2;1}$ and $C_{4;3}$ are irreducible, but $C_{4;1}$ and $C_{4;2}$ are reducible. By using Eq. (4.13) we find

$$C_{4;1}=C_{4;2}=(C_{2;1})^2.$$

Let us write each $C(\ )$ which appears in Eq. (4.11) as the product of an irreducible $C(\ )$ and irreducible C's, and then collect all the terms proportional to each irreducible $C(\ )$. We obtain a result of the form

$$\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle=M^{-1}\sum_n\sum_p{}^{\mathrm{irr}}(-1)^n \times C_{2n;p}(\alpha,\beta,\alpha-\beta)\zeta_{2n;p}(t), \quad (4.15)$$

where $\sum^{\mathrm{irr}}$ denotes the sum over irreducible diagrams only. The $\zeta_{2n;p}(t)$ depend on the values of the irreducible C's but are independent of α and β. Each $\zeta_{2n;p}(t)$ contains all (odd) powers of t which are $\geq 2n-1$, since each $C_{2n;p}(\alpha,\beta,\alpha-\beta)$ appears in reducible $C(\ )$'s of all orders $\geq 2n$. The $\zeta_{2n;p}(t)$ turn out to have simple expressions in terms of $\langle b^2\rangle$ and $G(t)$ which may be found by comparing the explicit power series for $\zeta_{2n;p}(t)$ and $G(t)$. However, the same result may be obtained more transparently by a variational procedure which provides certain dynamical insights.

There are $M(M-1)$ ϕ's, and only M sums $\sum_\beta C_{2n;p}(\alpha,\beta,\alpha-\beta)$ for given n and p. In the limit $M\to\infty$ it will be possible, therefore, to make wide classes of variations $\Delta\phi$ such that Eqs. (4.4) and (4.13) continue to hold and such that $\Delta C_{2n;p}=0$ for all finite n. Under these constraints, $\Delta\zeta_{2n;p}(t)=0$. Consequently, we have

$$\Delta\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle=M^{-1}\sum_n\sum_p{}^{\mathrm{irr}}(-1)^n\zeta_{2n;p}(t) \times\Delta C_{2n;p}(\alpha,\beta,\alpha-\beta). \quad (4.16)$$

Now consider a (finite) variation

$$\Delta\phi_{\alpha-\beta,-\beta,\alpha}=\Delta\phi_{\alpha,\beta,\alpha-\beta}{}^*$$

for a particular α and β, with all the other ϕ's fixed. We may vary the real and imaginary parts of $\phi_{\alpha-\beta,-\beta,\alpha}$ independently. Identical results are obtained by supposing $\phi_{\alpha-\beta,-\beta,\alpha}$ to vary while $\phi_{\alpha-\beta,-\beta,\alpha}{}^*=\phi_{\alpha,\beta,\alpha-\beta}$ is held fixed, and we shall adopt the latter procedure. Then, by Eqs. (4.12),

$$\Delta C_{2;1}(\alpha,\beta,\alpha-\beta)=\phi_{\alpha,\beta,\alpha-\beta}\Delta\phi_{\alpha-\beta,-\beta,\alpha}, \quad (4.17)$$

while from Eq. (4.13) we see that $\Delta C_{2n;p}=O(M^{-1})$ for all n and p. Thus the constraints stated previously are satisfied for $M\to\infty$. By Eq. (4.6), $G_{\alpha-\beta,\alpha}(t)$ satisfies

$$dG_{\alpha-\beta,\alpha}(t)/dt +iM^{-\frac{1}{2}}\sum_\sigma\phi_{\alpha-\beta,-\sigma,\alpha-\beta+\sigma}b_{-\sigma}G_{\alpha-\beta+\sigma,\alpha}(t)=0. \quad (4.18)$$

The effect of the variation $\Delta\phi_{\alpha-\beta,-\beta,\alpha}$ is to produce on the right-hand side of Eq. (4.18) the additional term

$$-iM^{-\frac{1}{2}}\Delta\phi_{\alpha-\beta,-\beta,\alpha}b_{-\beta}G_{\alpha,\alpha}(t)$$

which, we note, is $O(M^{-\frac{1}{2}})$. Now we recall that $G_{\alpha-\beta,\alpha}(t)$ is simply the amplitude $q_{\alpha-\beta}(t)$ under a particular initial condition at $t=0$. Therefore, to order $M^{-\frac{1}{2}}$, we have

$$\Delta G_{\alpha-\beta,\alpha}(t)=\int_0^t G_{\alpha-\beta,\alpha-\beta}(t-s) \times[-iM^{-\frac{1}{2}}\Delta\phi_{\alpha-\beta,-\beta,\alpha}b_{-\beta}G_{\alpha,\alpha}(s)]ds, \quad (4.19)$$

since $G_{\alpha-\beta,\alpha-\beta}$ is the diagonal response function for $q_{\alpha-\beta}$ and the perturbation does not affect the initial condition. [Note that $\Delta G_{\alpha,\alpha}(t)$ and $\Delta G_{\alpha-\beta,\alpha-\beta}(t)$ are $O(M^{-1})$ under our constraints.] On referring to Eq. (4.10), we obtain $\Delta\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle$ immediately. It is clear that our variation gives $\Delta C_{2n;p}(\alpha,\beta,\alpha-\beta)=O(M^{-1})$ for all irreducible diagrams with $n>1$. Then, by Eqs. (4.16) and (4.17), we find

$$\zeta_{2;1}(t)=\int_0^t\langle b_\beta b_{-\beta}G_{\alpha-\beta,\alpha-\beta}(t-s)G_{\alpha,\alpha}(s)\rangle ds \quad (4.20)$$

in the limit $M\to\infty$. As we have noted previously, $G_{\alpha,\alpha}(t)$ and $G_{\alpha-\beta,\alpha-\beta}(t)$ are statistically sharp in the limit. Therefore, by Eqs. (4.9) and (3.10),

$$\zeta_{2;1}(t)=\langle b^2\rangle\int_0^t G(t-s)G(s)ds. \quad (4.21)$$

The higher $\zeta_{2n;p}$ may be found by similar analysis based on more general variations. The result is

$$\zeta_{2n;p}=\langle b^2\rangle^n G(*G)^{2n-1}, \quad (4.22)$$

where $G(*G)^{2n-1}$ is a repeated convolution; e.g. (for argument t),

$$G(*G)^3=\int_0^t ds\int_0^s ds'\int_0^{s'} ds''G(t-s)G(s-s') \times G(s'-s'')G(s'').$$

On collecting the appropriate relations, we have the

final result

$$dG/dt=\sum_{n=1}^{\infty}\sum_{p}^{\text{irr}}(-1)^n C_{2n;p}\langle b^2\rangle^n G(*G)^{2n-1},$$
$$G(0)=1. \quad (4.23)$$

The value of this infinite-series integro-differential equation for $G(t)$ is that only the irreducible $C_{2n;p}$ appear explicitly.

5. RANDOM COUPLING MODEL

We shall now consider a particular stochastic assignment of the ϕ's. Let

$$\phi_{\alpha,\beta,\alpha-\beta}=\exp(i\theta_{\alpha,\beta,\alpha-\beta}), \quad (5.1)$$

where $\theta_{\alpha,\beta,\alpha-\beta}$ is real and satisfies

$$\theta_{\alpha-\beta,-\beta,\alpha}=-\theta_{\alpha,\beta,\alpha-\beta}. \quad (5.2)$$

For each choice of α and β, let $\theta_{\alpha,\beta,\alpha-\beta}$ take a value at random in the interval 0 to 2π, subject only to Eq. (5.2). The value must be the same, of course, for every realization in the ensemble. Now let $M\rightarrow\infty$. Clearly this assignment satisfies Eq. (4.4). In addition, it yields $|\phi_{\alpha,\beta,\alpha-\beta}|=1$, and, therefore, retains unaltered the *strengths* of the individual dynamical couplings of pairs q_α, $q_{\alpha-\beta}$ which characterize Eq. (3.6). Now, however, the *phases* of the couplings are completely unrelated for different pairs. We shall call the present choice the random coupling model.[14]

By referring to Eqs. (4.12) and (4.13), we find $C_{2;1}=1$, as in the true problem (all ϕ's unity). Consider $C_{4;3}$, however. Each product in the sum has modulus 1, but the phase of the product changes at random with β and γ. Consequently, $C_{4;3}=O(M^{-1})$. In a similar fashion, we see that the only $C_{2n;p}$ which survive in the limit are those in which the product of ϕ's consists entirely of conjugate pairs and which, therefore, are reducible to powers of $C_{2;1}$. Consequently, for $M\rightarrow\infty$,

$$C_{2;1}=1,$$
$$C_{2n;p}=0 \quad (n>1) \quad \text{(all irreducible diagrams)}. \quad (5.3)$$

It follows that Eq. (4.23) reduces to the closed form

$$dG/dt+\langle b^2\rangle G*G=0, \quad G(0)=1. \quad (5.4)$$

Equation (5.4) is readily solved by Laplace transformation. We find

$$G(t)=J_1(2b_*t)/b_*t, \quad (5.5)$$

$$\tilde{G}(\omega)=(\pi b_*)^{-1}[1-(\omega/2b_*)^2]^{\frac{1}{2}} \quad (|\omega|\leq 2b_*),$$
$$=0 \quad (|\omega|>2b_*), \quad (5.6)$$

where $b_*=\langle b^2\rangle^{\frac{1}{2}}$ as before. Considered as an approximation to Eqs. (2.8) and (2.7), the present results display a type of uniform validity which is absent in any finite stage of the iteration or cumulant-discard schemes discussed in Sec. 2. The spectral density of Eq. (5.6) is continuous, and Eqs. (2.4) and (2.5) are satisfied. All the derivatives of $\tilde{G}(\omega)$ exists at $\omega=0$ so that all the moments $\int_0^\infty t^n G(t)dt$ exist. Equations (2.8) and (5.5) are compared in Fig. 3.

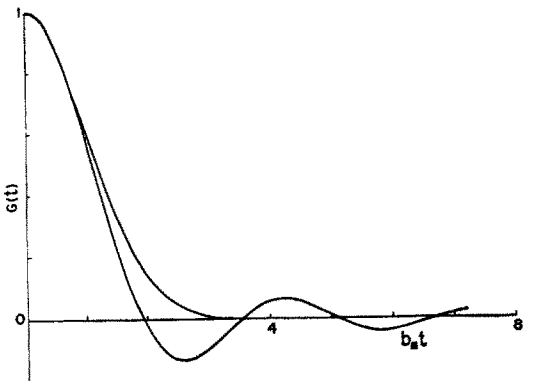

FIG. 3. Comparison of $G(t)$ for the true problem and the random coupling model.

It is important that certain of the properties just listed could have been predicted from the sole fact that Eq. (5.4) is an exact equation ($M\rightarrow\infty$) for a realizable ϕ assignment satisfying Eq. (4.4), and, hence, for a conservative dynamical problem. We recall that $G_{\alpha,\alpha}(t)=q_\alpha(t)$ when $q_\gamma(0)=\delta_{\alpha,\gamma}$ (all γ). But then

$$\sum_\gamma q_\gamma(0)q_\gamma^*(0)=1,$$

and, since $\sum_\gamma q_\gamma(t)q_\gamma^*(t)$ is a constant of motion, we have $|G_{\alpha,\alpha}(t)|\leq 1$, whence Eq. (2.5) readily follows. To establish Eq. (2.4), let us make, for each realization, a similarity transformation

$$q_\alpha(t)=\sum_\gamma B_{\alpha\gamma}q_\gamma'(t), \quad q_\gamma'(t)=\sum_\alpha B_{\gamma\alpha}^{-1}q_\alpha(t), \quad B_{\gamma\alpha}^{-1}=B_{\alpha\gamma}^*$$

($B_{\alpha\gamma}$ independent of t) such that Eq. (4.1) is brought to the diagonal form

$$dq_\gamma'(t)/dt+i\omega_\gamma q_\gamma'(t)=0. \quad (5.7)$$

Since $\sum_\gamma q_\gamma'q_\gamma'^*=\sum_\alpha q_\alpha q_\alpha^*$ is a constant of motion, the ω_γ are real. Now if $G_{\gamma,\epsilon}'(t)$ is the response matrix of the new variables, $G_{\gamma,\epsilon}'(t)=\delta_{\gamma,\epsilon}\exp(-i\omega_\gamma t)$, and, therefore,

$$G_{\alpha,\alpha}(t)=\sum_{\gamma,\epsilon}B_{\alpha\gamma}G_{\gamma,\epsilon}'(t)B_{\epsilon\alpha}^{-1}=\sum_\gamma B_{\alpha\gamma}B_{\alpha\gamma}^*\exp(-i\omega_\gamma t).$$

Hence $\tilde{G}_{\alpha,\alpha}(\omega)$ is real and nonnegative in each realization, which implies Eq. (2.4). Finally, we note that the model problem resulting from a general realizable ϕ assignment involves the interaction of an infinite number of degrees of freedom q_α when $M\rightarrow\infty$. From this, and the fact that the b_α are continuously distributed over the ensemble, we may anticipate that $\tilde{G}(\omega)$ exhibits a continuous or band structure and that $G(t)\rightarrow 0$, $t\rightarrow\infty$.

It is possible to understand qualitatively why the complex detailed dynamics of the random coupling

[14] This model is unrelated to the "random phase approximation" [D. Pines and D. Bohm, Phys. Rev. 85, 338 (1952)]. We make no assumption about the phases of the q_α themselves.

model lead to a simplification of the statistical dynamics and to closure of Eq. (4.23). The function $\langle G_{\alpha,\alpha}(t)\rangle$ describes the decay of q_α due to transfer of an initial excitation, amplitude $q_\alpha(0)=1$, to the rest of the degrees of freedom. In general, the decay requires that certain phase relations be set up between q_α and the other amplitudes. A phase relation between q_α and $q_{\alpha-\beta}$ can arise either from direct dynamical coupling (involving the coupling coefficients $-iM^{-\frac{1}{2}}\phi_{\alpha,\beta,\alpha-\beta}b_\beta$ and $-iM^{-\frac{1}{2}}\phi_{\alpha-\beta,-\beta,\alpha}b_{-\beta}$) or from indirect coupling through chains of other modes q_γ. In fact, each term in the irreducible diagram expansion Eq. (4.15) may be regarded as describing the transfer of excitation from q_α to $q_{\alpha-\beta}$ along the chain of intermediate modes represented by the directed solid line segments in the associated diagram. The closing of the solid line on itself then represents the reaction on mode α and the consequent diminution of q_α. The factors G, whose repeated convolution yields the $\zeta_{2n;p}$, incorporate the effect of the dynamical interaction as a whole on the transfer process. This effect is to relax the phase relations set up along the chain.

In the random coupling model, only the direct interaction, associated with $C_{2;1}$, is effective in the transfer of excitation. The contributions associated with the indirect paths of interaction cancel, when summed over all possible intermediate modes, because of the random phases of the ϕ's. The coupling of q_α and $q_{\alpha-\beta}$ to all the rest of the modes, therefore, affects $\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle$ only by relaxing the phase relations induced by the direct interaction of these two modes.

All $C_{2n;p}$ which are expressible as powers of $C_{2;1}$ have the value unity in the random coupling model, and all other $C_{2n;p}$ vanish. Thus we see from Eq. (4.14) that the power series for the model $G(t)$ consists of a particular subset of terms of all orders from the corresponding series for the true problem (all $C_{2n;p}$ unity). The terms retained are all those whose associated diagrams can be reduced to that for $C_{2;1}$ (Fig. 2) by by iterating any number of times, on any solid lines, the contraction operation shown in Fig. 4(a). Examples of included diagrams are shown in Fig. 4(b). It follows readily from Eq. (5.5) that the number of diagrams of this type with $2n$ vertices is

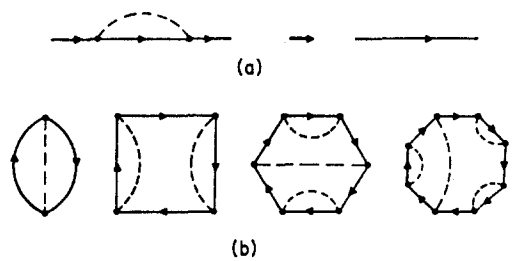

FIG. 4. (a) Contraction operation for the random coupling model; (b) typical diagrams included in the random coupling model. (Any vertex may be taken as the fixed vertex.)

$$(-1)^n\left\{\frac{d^{2n}}{(dt)^{2n}}\left[\frac{J_1(2t)}{t}\right]\right\}_{t=0}.$$

6. INADMISSIBLE HIGHER APPROXIMATIONS

For the true problem (all $C_{2n;p}=1$), Eq. (4.23) reads

$$dG/dt=\sum_{n=1}^{\infty}(-1)^n S_{2n}\langle b^2\rangle^n G(*G)^{2n-1},\quad G(0)=1,\qquad (6.1)$$

where S_{2n} is the number of irreducible diagrams of order $2n$. The first few S_{2n} are $S_2=1$, $S_4=1$, $S_6=4$, $S_8=27$.[15] The relative success of Eq. (5.4) as an approximation to Eq. (6.1) suggests that we seek higher approximations satisfying equations of the form

$$dG/dt=\sum_{n=1}^{R}(-1)^n S_{2n}\langle b^2\rangle^n G(*G)^{2n-1},\quad G(0)=1\quad (R>1),\qquad (6.2)$$

which we obtain by giving all irreducible $C_{2n;p}$ the value one, $n\leq R$, and the value zero, $n>R$. One property of Eq. (6.2) can be predicted immediately. We recall that Eq. (4.23) represents simply a consolidation of Eq. (4.14). The present sums $\sum_p C_{2n;p}$ (reducible and irreducible diagrams included) clearly do not exceed the corresponding sums in the true problem. Since Eq. (2.10), which constitutes Eq. (4.14) for that problem, is absolutely convergent for all t, it follows that the power series expansions of the solutions of Eq. (6.2) are absolutely convergent for all t.

Nevertheless, these solutions are not valid higher approximations to Eq. (2.8). The reason is that the functions to which their expansions converge become infinite as $t\rightarrow\infty$. None of them, therefore, constitutes a uniform approximation, and for none of them does $\tilde{G}(\omega)$ exist. We shall illustrate this for $R=2$. If $\mathbf{G}(p)$ denotes the Laplace transform of $G(t)$, then Eq. (6.2) for this case is equivalent to

$$p\mathbf{G}(p)=1-\langle b^2\rangle[\mathbf{G}(p)]^2+\langle b^2\rangle^2[\mathbf{G}(p)]^4.\qquad (6.3)$$

Let us assume tentatively that $\mathbf{G}(0)=\int_0^\infty G(t)dt$ is finite. Then

$$[\mathbf{G}(0)]^2=[1\pm(-3)^{\frac{1}{2}}]/2\langle b^2\rangle,\qquad (6.4)$$

which is inconsistent with the reality of $G(t)$. Therefore, $\int_0^\infty G(t)dt$ cannot be finite. Further analysis readily shows that, for real ω, Eq. (6.3) is inconsistent with $\mathrm{Re}\,\{\mathbf{G}(-i\omega)\}=0(\omega^{-r})$, $\omega\rightarrow 0$, if r is any finite power. It follows that $G(t)$ grows faster than any power of t as $t\rightarrow\infty$.

The numerical solutions of Eq. (6.2) for several values of R are compared with Eq. (2.8) in Fig. 5. As R increases, it will be noted that the approximations increase in accuracy for small t but diverge faster at large t. In this respect, our present results resemble very closely those of truncating the original power series

[15] In general, $S_{2n}\neq(n-1)^{n-1}$.

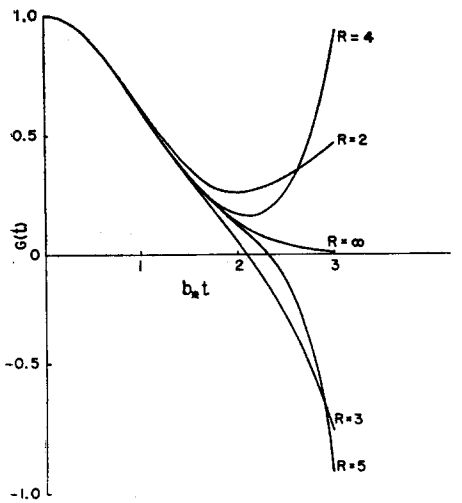

FIG. 5. Solutions of Eq. (6.2) compared with $G(t)$ for the true problem ($R=\infty$).

Eq. (2.10) after a finite number of terms. They do not appear to represent a significant improvement over the latter.

The failure of the present approximations has an immediate interpretation. Divergence of $G(t)$ as $t \to \infty$ is inconsistent with Eq. (2.5). It follows that the values of the irreducible C's implied by Eq. (6.2) are not realizable by any assignment of the ϕ's consistent with Eq. (4.4). Thus these approximations do not correspond to any dynamical model in our sense.[16]

If we regard a stochastic assignment of the $\phi_{\alpha,\beta,\alpha-\beta}$ for $M \to \infty$ as a distribution over the set of index values α and β, then the $C_{2n;p}$ are moments of this distribution and there are an infinite set of realizability inequalities which they must satisfy. The values $C_{2;1}=1$, $C_{2n;p}=0$ (all higher irreducible diagrams) for the random coupling model correspond to complete statistical independence of the $\phi_{\alpha,\beta,\alpha-\beta}=\phi_{\alpha-\beta,-\beta,\alpha}{}^*$ in this sense. Nonvanishing values for the higher irreducible C's imply statistical correlation among the ϕ's.

The nature of realizability inequalities for simpler statistical problems suggests that, when $C_{2;1}=1$, a wide choice of realizable nonzero values can be given to the higher irreducible $C_{2n;p}$, provided these values are small enough. Let us consider the assignment

$$C_{2;1}=1, \quad C_{4;3}=a, \quad C_{2n;p}=0 \quad \text{(all higher irreducible diagrams)}, \tag{6.5}$$

where a is a real constant. For $a=1$ this gives Eq. (6.2), $R=2$. Instead of Eq. (6.3), we now find, in the general case,

$$p\mathbf{G}(p)=1-\langle b^2\rangle[\mathbf{G}(p)]^2+a\langle b^2\rangle^2[\mathbf{G}(p)]^4, \tag{6.6}$$

whence

$$[\mathbf{G}(0)]^2=[1-(1-4a)^{\frac{1}{2}}]/2a\langle b^2\rangle. \tag{6.7}$$

Equation (6.6) yields real, nonnegative $\tilde{G}(\omega)$ for all ω if

$$-\tfrac{1}{12} \leq a \leq \tfrac{1}{4}, \tag{6.8}$$

which suggests that Eq. (6.8) may represent the range of realizability of Eq. (6.5). In Fig. 6, the solution $\tilde{G}(\omega)=\pi^{-1}\,\mathrm{Re}\{\mathbf{G}(-i\omega)\}$ on the relevant branch of Eq. (6.6) is compared, for several values of a, with Eqs. (2.7) and (5.6). It will be noted that the form of $\tilde{G}(\omega)$ changes continuously with a up to the limit $a=\frac{1}{4}$, where the slope at $\omega=0$ changes abruptly from 0 to ∞. It is apparent that none of the present approximations represents a substantial improvement over the random coupling solution ($a=0$). For $a<0$, the form of $\tilde{G}(\omega)$ changes continuously with a down to the limit $a=-\frac{1}{12}$; there, a singularity appears at the cutoff point of the spectrum. We conclude tentatively, lacking contrary evidence, that Eq. (6.8) does represent the range of realizability of Eq. (6.5).

The results of the present section suggest that great caution be exercised in carrying out partial summations of diagrams in the power series expansion for $G(t)$. It is by no means true that the more terms summed, the better the approximation. Our inadmissible approximation Eq. (6.2) ($R=2$) is equivalent to the retention, in Eq. (4.14) for the true problem, of all terms whose diagrams can be reduced to the diagram for $C_{2;1}$ by iterated application, on any solid lines, of the contraction operations shown in Fig. 7(a). Examples are shown in Fig. 7(b). Thus, the terms retained are selected according to well-defined and plausible topological properties of the diagrams. Moreover, as we have noted, in the t domain they constitute an absolutely convergent subseries of an absolutely convergent series.

It will have been recognized by this point that the diagram summations we have employed are intimately

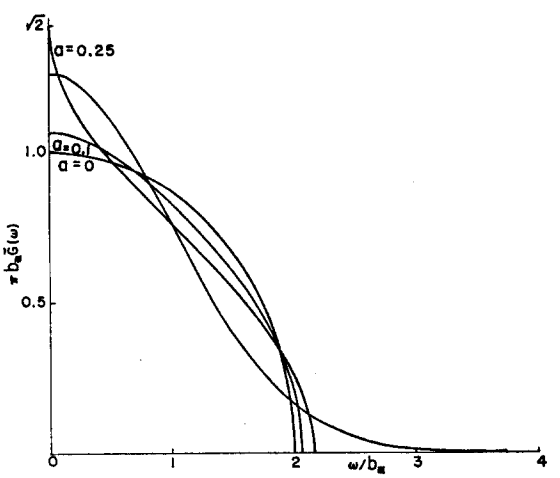

FIG. 6. Solutions $\tilde{G}(\omega)$ of Eq. (6.6) for several values of a compared with $\tilde{G}(\omega)$ for the true problem.

[16] The relations between irreducible and reducible C's, to which we have appealed in discussing Eq. (6.2), are not affected by the unrealizability of the C's. These relations may be regarded here as formal implications of the requirement that Eq. (4.14) agree with the power series for $G(t)$ obtained by the iteration solution of Eq. (4.23).

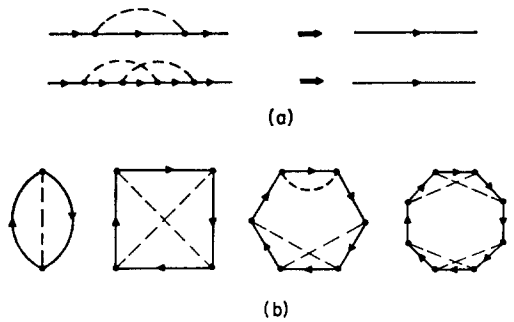

FIG. 7. (a) Contraction operations for Eq. (6.2) with $R=2$; (b) typical diagrams included by Eq. (6.2) with $R=2$.

related to summations of perturbation series terms in quantum field theory and quantum statistical mechanics. Our present results suggest that caution be exercised in these problems also. There too, it is possible that plausible-appearing and summable classes of diagrams are better omitted than included. We hope to return to these questions in a later paper.

7. SECOND STOCHASTIC MODEL

The results of the last section emphasize the desirability of seeking higher approximations to Eq. (6.1) which correspond to realizable values of the C's. We shall now describe a second stochastic model for which $\tilde{G}(\omega)$ satisfies Eq. (2.4) and is substantially closer to Eq. (2.7) than is the random coupling result. Consider the contraction operation shown in Fig. 8(a). Each application of it to a diagram reduces the number of vertices by two. Let us take $C_{2;1}=1$ and assign the value a^{n-1} to all irreducible $C_{2n;p}$ whose diagrams can be transformed into that for $C_{2;1}$ by $n-1$ applications, anywhere, of this operation. These diagrams represent an infinite subset of the terms in Eq. (4.23). [Examples are shown in Fig. 8(b).] Let us assign the value zero to all other irreducible $C_{2n;p}$. [Examples are shown in Fig. 8(c).] Now let us take $a=1$. Clearly this implies the value 1, as in the true problem, for all reducible and irreducible $C_{2n;p}$ whose diagrams can be transformed into that for $C_{2;1}$ by repeated application of the line operation of Fig. 4(a) and the vertex operation of Fig. 8(a). All other $C_{2n;p}$ have the value zero.

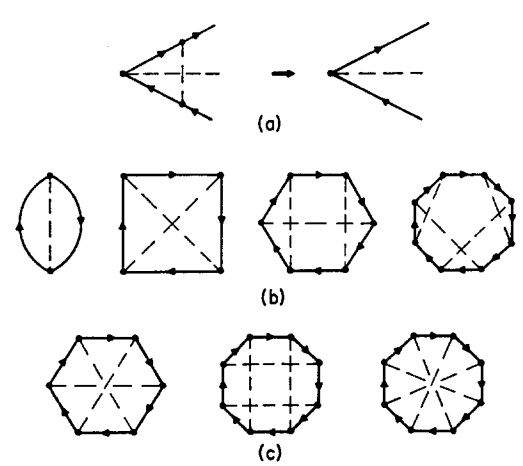

FIG. 8. (a) Contraction operation for the second stochastic model; (b), (c) typical diagrams included and excluded, respectively, in the second stochastic model.

We have not found an explicit construction for this model of the type provided by Eq. (5.1), *et seq.*, for the random coupling model. Consequently, we have no proof of realizability. As we shall see, however, examination of the dependence of $\tilde{G}(\omega)$ on a, in analogy to Sec. 6, suggests that the model is realizable.

Since the present model retains an infinite subset of terms in Eq. (4.23), it does not directly yield a closed equation for $G(t)$. However, we can obtain a closed system [Eqs. (7.6) and (7.17)] by considering simultaneously the first two equations of an hierarchy analogous to Eq. (2.11). Let

$$H(t)\equiv\sum_\beta\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle=dG(t)/dt.$$

From Eq. (4.6) we find

$$dH(t)/dt=-\sum_\beta\phi_{\alpha,\beta,\alpha-\beta}\phi_{\alpha-\beta,-\beta,\alpha}\times\langle b_\beta b_{-\beta}G_{\alpha,\alpha}(t)\rangle+J(t),\quad H(0)=0,\quad(7.1)$$

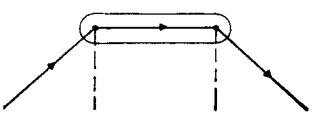

FIG. 9. Fixed diagram part for $J(t)$.

where

$$J(t)=-M^{-1}\sum_{\beta,\gamma}^{(\gamma\neq-\beta)}\phi_{\alpha,\beta,\alpha-\beta}\phi_{\alpha-\beta,\gamma,\alpha-\beta-\gamma}\times\langle b_\beta b_\gamma G_{\alpha-\beta-\gamma,\alpha}(t)\rangle.\quad(7.2)$$

Since $G_{\alpha,\alpha}(t)$ is statistically sharp ($M\to\infty$), it follows from previous relations that the first term on the right-hand side of Eq. (7.1) may be rewritten $-C_{2;1}\langle b^2\rangle G(t)$. Hence, when $C_{2;1}=1$, we have the equations

$$\begin{aligned}dG(t)/dt&=H(t),\quad G(0)=1,\\ dH(t)/dt&=-\langle b^2\rangle G(t)+J(t),\quad H(0)=0.\end{aligned}\quad(7.3)$$

By Eq. (4.23) we have

$$H=\sum_{n=1}^{\infty}\sum_{p}^{\text{irr}}(-1)^nC_{2n;p}\langle b^2\rangle^nG(*G)^{2n-1}.\quad(7.4)$$

An analogous expansion for $J(t)$ may be found by analysis very similar to that which leads to Eq. (4.23). The result is

$$J=\sum_{n=2}^{\infty}\sum_{p}^{J}(-1)^nC_{2n;p}\langle b^2\rangle^nG(*G)^{2n-2},\quad(7.5)$$

where $\sum^J$ is defined as follows: Construct a diagram part as shown in Fig. 9. Call it the fixed part. [The two vertices correspond to the two ϕ factors which appear

explicitly in Eq. (7.2).] The summation $\sum^J$ then is over every closed diagram, constructed by combining two or more vertices with the fixed part, that contains no part, wholly external to the fixed part, which is connected to the rest of the diagram by only solid lines. The three simplest diagrams included are shown in Fig. 10. It will be noted that $\sum^J$ contains both reducible and irreducible diagrams in the sense of Sec. 4. The reducible diagrams all resemble Fig. 10(a) in that the associated C is the product of just two irreducible C's.

Let us denote by Fig. 11(a) the totality of possible diagram parts, with the two solid and single dashed external lines shown, that can be transformed into a single vertex by repeated contractions as shown in Fig. 8(a). Let us call this structure a consolidated vertex part. Then we may represent the entire class of irreducible diagrams which contribute to $H(t)$, in the present model, by the single consolidated diagram shown in Fig. 11(b).[17] In a similar fashion, we may represent by consolidated diagrams all the contributions to $J(t)$ in the present model.[17a] Clearly, two consolidated diagrams included are those shown in Figs. 12(a) and 12(b). If we independently replace the several consolidated vertex parts in these diagrams by all possible

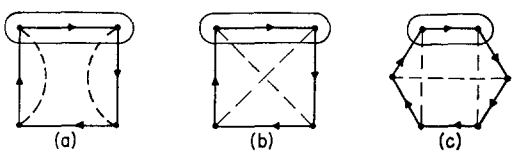

FIG. 10. The simplest diagrams contributing to $J(t)$.

diagram parts which they represent, then we obtain all the individual contributing diagrams which are contractible into Figs. 10(a) or 10(b), respectively. The required contractions do not involve the fixed part. It can be seen that all other diagrams contributing in the present model are represented by the infinite class of consolidated diagrams indicated in Fig. 12(c). These diagrams all may be transformed into that for $C_{2;1}$ by sequences of contractions which now involve the fixed part.

As the representation by consolidated diagrams suggests, the present model leads to a closed expression for $J(t)$ in terms of $H(t)$ and $G(t)$. It is convenient at this point to work with the Laplace transform representation. If $\mathbf{G}(p)$, $\mathbf{H}(p)$, and $\mathbf{J}(p)$ denote the respective transforms of $G(t)$, $H(t)$, and $J(t)$, then the transforms of Eqs. (7.3)–(7.5) are[18]

[17] It is easy to see that any diagram which is transformable into the diagram for $C_{2;1}$ by contraction operations which involve the fixed vertex may also be so transformed by an alternative sequence of contractions which do not involve this vertex. Thus the diagrams included in this consolidated diagram are exhaustive. (a) Our "consolidated" diagrams are "irreducible" diagrams in the terminology of quantum field theory.

[18] The argument p in $\mathbf{G}(p)$, etc., should not be confused with the index p in $C_{2n;p}$.

FIG. 11. (a) Consolidated vertex part; (b) the consolidated diagram for $H(t)$.

$$p\mathbf{G}(p)=1+\mathbf{H}(p), \quad p\mathbf{H}(p)=-\langle b^2\rangle\mathbf{G}(p)+\mathbf{J}(p), \tag{7.6}$$

$$\mathbf{H}(p)=\sum_{n=1}^{\infty}\sum_{p}^{\text{irr}}(-1)^n C_{2n;p}\langle b^2\rangle^n[\mathbf{G}(p)]^{2n}, \tag{7.7}$$

$$\mathbf{J}(p)=\sum_{n=2}^{\infty}\sum_{p}^{J}(-1)^n C_{2n;p}\langle b^2\rangle^n[\mathbf{G}(p)]^{2n-1}. \tag{7.8}$$

Let us write

$$\mathbf{J}(p)=\mathbf{J}^{(1)}(p)+\mathbf{J}^{(2)}(p)+\mathbf{J}^{(3)}(p), \tag{7.9}$$

where $\mathbf{J}^{(1)}(p)$, $\mathbf{J}^{(2)}(p)$, and $\mathbf{J}^{(3)}(p)$ are the contributions associated with Figs. 12(a), 12(b), and 12(c), respectively. It can be seen with the aid of the diagrams that the terms of Eq. (7.8) included in $\mathbf{J}^{(1)}(p)$ are in one-to-one correspondence to the totality of terms in the expansion

$$[\mathbf{H}(p)]^2=\sum_{n,m}\sum_{p,q}^{\text{irr}}(-1)^{n+m}C_{2n;p}C_{2m;q}\langle b^2\rangle^{n+m}\times[\mathbf{G}(p)]^{2n+2m}, \tag{7.10}$$

which follows from Eq. (7.7). On evaluating the corresponding terms by means of the rule $C_{2n;p}=a^{n-1}$ (all nonvanishing irreducible C's) and then summing, we readily find

$$\mathbf{J}^{(1)}(p)=[\mathbf{G}(p)]^{-1}[\mathbf{H}(p)]^2. \tag{7.11}$$

A similar correspondence exists for $\mathbf{J}^{(2)}(p)$, and we thereby find

$$\mathbf{J}^{(2)}(p)=a[\mathbf{G}(p)]^{-1}[\mathbf{H}(p)]^2. \tag{7.12}$$

The evaluation of $\mathbf{J}^{(3)}(p)$ is somewhat more involved. Let us write

$$\mathbf{J}^{(3)}(p)=\sum_{i=1}^{\infty}\mathbf{J}^{(3,i)}(p), \tag{7.13}$$

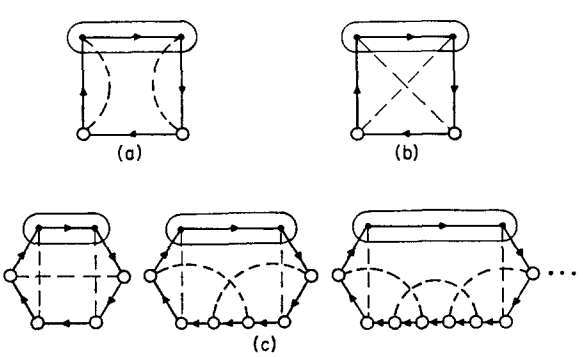

FIG. 12. Consolidated diagrams contributing to $J(t)$ in the second stochastic model.

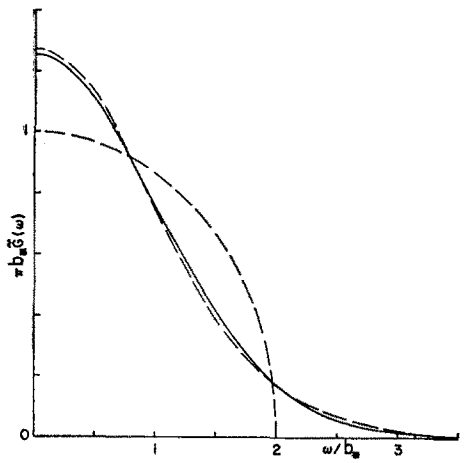

FIG. 13. Comparison of $\tilde{G}(\omega)$ for the random coupling model and the second stochastic model (dashed curves) with $\tilde{G}(\omega)$ for the true problem.

where $\mathbf{J}^{(3,i)}(p)$ is the contribution from the ith consolidated diagram in the sequence of Fig. 12(c). The series for $\mathbf{J}^{(3,1)}(p)$ is in one-to-one correspondence with that for $[\mathbf{H}(p)]^4$, and we find

$$\mathbf{J}^{(3,1)}(p) = -a^2\langle b^2\rangle^{-1}[\mathbf{G}(p)]^{-3}[\mathbf{H}(p)]^4 \quad (7.14)$$

by comparing corresponding terms. In a similar fashion, comparing the series for $\mathbf{J}^{(3,i+1)}(p)$ and $[\mathbf{H}(p)]^2\mathbf{J}^{(3,i)}(p)$, we find

$$\mathbf{J}^{(3,i+1)}(p) = -a\langle b^2\rangle^{-1}[\mathbf{G}(p)]^{-2}[\mathbf{H}(p)]^2\mathbf{J}^{(3,i)}(p), \quad (7.15)$$

whence,

$$\mathbf{J}^{(3)}(p) = \mathbf{J}^{(3,1)}(p) - a\langle b^2\rangle^{-1}[\mathbf{G}(p)]^{-2}[\mathbf{H}(p)]^2\mathbf{J}^{(3)}(p). \quad (7.16)$$

On combining our results (and suppressing the argument p) we have, finally,

$$\mathbf{J} = \mathbf{G}^{-1}\mathbf{H}^2\{1+[a/(1+a\langle b^2\rangle^{-1}\mathbf{G}^{-2}\mathbf{H}^2)]\}. \quad (7.17)$$

Eliminating $\mathbf{H}$ and $\mathbf{J}$ from Eqs. (7.6) and (7.17), we obtain

$$\langle b^2\rangle^2\mathbf{G}^4 + p(\langle b^2\rangle + ap^2)\mathbf{G}^3 - (\langle b^2\rangle + 3ap^2)\mathbf{G}^2 + 3ap\mathbf{G} - a = 0. \quad (7.18)$$

The relevant branch of Eq. (7.18) is the one for which $\tilde{G}(\omega) = \pi^{-1}\,\mathrm{Re}\{\mathbf{G}(-i\omega)\}$ reduces to Eq. (5.6) when $a=0$, and it is easily verified that such a branch exists. Let us examine the behavior of $\tilde{G}(\omega)$ on this branch as a is varied. For sufficiently small a, it is plausible to assume that our assignment of values to the C's is realizable. As we increase a, we may plausibly anticipate that $\tilde{G}(\omega)$ will begin to violate Eq. (2.4), or at least will exhibit some discontinuous change in its dependence on a, when a critical value is reached for which the C's are unrealizable by any assignment of values to the ϕ's consistent with Eq. (4.4). This argument is supported by the example of Sec. 6.

The behavior of Eq. (7.18) is accessible by standard techniques for quartic equations. One finds that the form of $\tilde{G}(\omega)$ on the branch of interest varies continuously with a for $-\frac{1}{4} < a < \infty$. Over this range,

$$\tilde{G}(0) = (\sqrt{2}\pi b_*)^{-1}[1+(1+4a)^{\frac{1}{2}}]^{\frac{1}{2}}, \quad (7.19)$$

and, for $a>0$, $\tilde{G}(\omega)$ decreases monotonically with increase of ω^2 up to a cutoff frequency given by

$$\omega_c^2 = \tfrac{1}{2}a^{-1}s^{-2}(1+s)^2[1-(1-4as)^{\frac{1}{2}}]\langle b^2\rangle, \quad (7.20)$$

where

$$s = 2-(1+a^{-1}+D^{\frac{1}{2}})^{\frac{1}{2}}-(1+a^{-1}-D^{\frac{1}{2}})^{\frac{1}{2}},$$
$$D = (1+a^{-1})^2-(1-\tfrac{2}{3}a^{-1})^3.$$

As a increases, ω_c^2 increases monotonically. For $a<-\frac{1}{4}$, $\tilde{G}(0)$ is complex, and we conclude that this gives a lower bound to the range of realizability. There appears to be no upper bound, at least on the basis of the present considerations.

The properties just listed appear to justify the tentative conclusion that the present model is realizable for $a=1$. It should be emphasized, however, that the arguments given do not constitute a proof of realizability. The latter would require an explicit prescription for constructing ϕ's which yield the model. We have not found such a prescription, and, therefore, we regard the investigation of the present model as incomplete.

The function $\tilde{G}(\omega)$ for $a=1$ is compared in Fig. 13 with Eqs. (5.6) and (2.7). It will be noted that the present model gives a close approximation to Eq. (2.7) and represents a substantial improvement over the random coupling model.

The apparent realizability of the present model, and the significant improvement it gives over the random coupling model, suggest that there may be an infinite sequence of closed realizable stochastic models in which successively broader classes of irreducible C's are given the value one and such that $G(t)$ converges rapidly to its value in the true problem. If so, the coupling coefficients $A_{[n,r,s]}$ in Eq. (4.2) may exhibit a distribution, as functions of n, r, and s, which clusters more and more closely about the diagonal values $A_{[n,r,s]} = \delta_{r,n}\delta_{s,n}$ as one ascends the sequence. Thus we may hope that any given dynamical properties of the models should converge in a statistical sense to those of the original collection of uncoupled oscillators. The analytical complexity of models higher than the two already described is formidable.

8. DRIVEN RANDOM OSCILLATOR

Let us add to the right-hand side of Eq. (4.2) a forcing term $f_{[n]}(t)$ which is identically distributed for each n, statistically independent for different n, and statistically independent of $b_{[r]}$ for all n and r. Let us take the initial conditions

$$q_{[n]}(t_0) = 0. \quad (8.1)$$

On writing

$$f_{[n]}(t) = \bar{f}(t) + f_{[n]}'(t), \quad \bar{f}(t) \equiv \langle f_{[n]}(t)\rangle, \quad (8.2)$$

and introducing collective forces $f_\alpha(t)$ defined in correspondence to Eq. (3.1), we find

$$\langle M^{-\frac{1}{2}}f_0(t)\rangle=\bar{f}(t),\quad \langle|M^{-\frac{1}{2}}f_0(t)-\bar{f}(t)|^2\rangle=O(M^{-1}),$$
$$\langle f_\alpha(t)\rangle=0,\quad \langle f_\alpha(t)f_\beta^*(t')\rangle=\delta_{\alpha,\beta}F(t,t')\quad(\alpha\neq0), \tag{8.3}$$

where

$$F(t,t')=\langle f_{[n]}'(t)f_{[n]}'^*(t')\rangle.$$

We see that $f_0(t)$ plays a special role: When $M\to\infty$, the quantity $M^{-\frac{1}{2}}f_0(t)=M^{-1}\sum_n f_{[n]}(t)$ takes the sharp value $\bar{f}(t)$. It is easily verified that $f_\alpha(t)$ depends only on the $f_{[n]}'(t)$ if $\alpha\neq0$.

In place of Eq. (4.1) we now have

$$dq_\alpha(t)/dt=-iM^{-\frac{1}{2}}\textstyle\sum_\beta\phi_{\alpha,\beta,\alpha-\beta}b_\beta q_{\alpha-\beta}(t)+f_\alpha(t). \tag{8.4}$$

Suppose that Eq. (8.4) is formally integrated from t_0 and solved by iteration. By arguments similar to those which give Eq. (4.7), we find

$$\langle q_\alpha(t)\rangle=0\quad(\alpha\neq0),\quad \langle q_\alpha(t)q_\gamma^*(t')\rangle=0\quad(\alpha\neq\gamma). \tag{8.5}$$

By Eqs. (8.5) and (3.3) we have, for all n,

$$\langle q_{[n]}(t)\rangle=\bar{q}(t),\quad \bar{q}(t)\equiv\langle M^{-\frac{1}{2}}q_0(t)\rangle. \tag{8.6}$$

It may be verified from a term-by-term examination of the iteration solution that the variance of $M^{-\frac{1}{2}}q_0(t)=M^{-1}\sum_n q_{[n]}(t)$ is $O(M^{-1})$. Thus, $M^{-\frac{1}{2}}q_0(t)$ is statistically sharp $(M\to\infty)$ and may be identified with $\bar{q}(t)$.[19]

Because of the special role played by $q_0(t)$, it is convenient to impose, in addition to Eqs. (4.4) and (4.13), the condition[20]

$$\phi_{\mu,\lambda,\sigma}=1\quad(\mu\text{ or }\sigma=0). \tag{8.7}$$

Then from Eq. (8.4), we obtain $(M\to\infty)$

$$d\bar{q}(t)/dt+iM^{-1}\textstyle\sum_\beta'\langle b_{-\beta}q_\beta(t)\rangle=\bar{f}(t), \tag{8.8}$$

$$dq_\alpha(t)/dt=-ib_\alpha\bar{q}(t)-iM^{-\frac{1}{2}}\textstyle\sum_\beta'\phi_{\alpha,\alpha-\beta,\beta}\times b_{\alpha-\beta}q_\beta(t)+f_\alpha(t)\quad(\alpha\neq0), \tag{8.9}$$

where $\sum_\beta'$ implies that $\beta=0$ is excluded.

Let us write

$$q_{[n]}(t)=\bar{q}(t)+q_{[n]}'(t), \tag{8.10}$$

where, by Eq. (8.6), $\langle q_{[n]}'(t)\rangle=0$. We shall call $\bar{q}(t)$ and $q_{[n]}'(t)$ the "coherent" and "incoherent" amplitudes, respectively. An explicit solution for $\bar{q}(t)$ is readily obtained. From the definition of the response matrix, and the statistical independence of the f's and the b's, we have

$$\langle q_0(t)\rangle=\sum_\alpha\int_{t_0}^t\langle G_{0,\alpha}(t-s)f_\alpha(s)\rangle ds=\sum_\alpha\int_{t_0}^t\langle G_{0,\alpha}(t-s)\rangle\langle f_\alpha(s)\rangle ds,$$

whence, by Eqs. (8.3), (8.6), and (4.9), we obtain

$$\bar{q}(t)=\int_{t_0}^t G(t-s)\bar{f}(s)ds. \tag{8.11}$$

Consider now the covariance of the incoherent amplitude. Let

$$Q_{[n,m]}(t,t')=q_{[n]}'(t)q_{[m]}'^*(t'),\quad Q_{\alpha,\gamma}(t,t')=q_\alpha(t)q_\gamma^*(t').$$

On using Eqs. (3.3), (8.5), and (8.6), we find

$$\langle Q_{[n,m]}(t,t')\rangle=M^{-1}\textstyle\sum_\alpha'\exp[-i2\pi(n-m)\alpha/M]\times\langle Q_{\alpha,\alpha}(t,t')\rangle+O(M^{-1}). \tag{8.12}$$

Therefore, if $\langle Q_{\alpha,\alpha}(t,t')\rangle$ is independent of α $(\alpha\neq0)$, we have $(M\to\infty)$

$$\langle Q_{[n,m]}(t,t')\rangle=\delta_{n,m}Q(t,t'),\qquad Q(t,t')=\langle Q_{\alpha,\alpha}(t,t')\rangle\quad(\alpha\neq0). \tag{8.13}$$

Let us assume hereafter that Eq. (8.13) holds. As we shall see shortly, this will be the case when Eqs. (4.13) and (8.7) are satisfied.

An important statistical property is

$$\langle b_\beta b_{-\beta}\cdots b_\mu b_{-\mu}Q_{\alpha,\alpha}(t,t')\rangle-\langle b^2\rangle\cdots\langle b^2\rangle Q(t,t')=O(M^{-1}),\quad(\alpha\neq0,\ |\alpha|\neq|\beta|\neq\cdots\neq|\mu|). \tag{8.14}$$

For the case of uncoupled oscillators (all ϕ's$=1$) this follows directly from Eq. (3.1) and the statistical independence of $b_{[n]}$, $q_{[n]}(t)$ and $b_{[r]}$, $q_{[r]}(t)$ for $n\neq r$. In the general case, it may be verified for each term of the iteration expansion of the left side of Eq. (8.14).[19]

From Eq. (8.9) we have

$$\partial Q(t,t')/\partial t=S(t,t')+S_C(t,t')+S_F(t,t'), \tag{8.15}$$

where

$$S(t,t')=\textstyle\sum_\beta'\langle S_{\alpha,\alpha-\beta,\beta}(t,t')\rangle\quad(\alpha\neq0),$$
$$S_{\alpha,\alpha-\beta,\beta}(t,t')=-iM^{-\frac{1}{2}}\phi_{\alpha,\alpha-\beta,\beta}b_{\alpha-\beta}q_\beta(t)q_\alpha^*(t'), \tag{8.16}$$
$$S_C(t,t')=-i\langle b_\alpha q_\alpha^*(t')\rangle\bar{q}(t)\quad(\alpha\neq0), \tag{8.17}$$
$$S_F(t,t')=\langle q_\alpha^*(t')f_\alpha(t)\rangle\qquad(\alpha\neq0). \tag{8.18}$$

Our notation anticipates the fact that the expressions given for $S(t,t')$, $S_C(t,t')$, and $S_F(t,t')$ are individually independent of α. It should be noted that the similar equation for $\partial Q(t,t')/\partial t'$ is redundant with Eq. (8.15) because of the property

$$Q(t,t')=Q^*(t',t), \tag{8.19}$$

which follows from the definition of $Q(t,t')$.

The quantity $S_F(t,t')$ is readily evaluated by an argument similar to that which gave Eq. (8.11). We have

$$\langle q_\alpha^*(t')f_\alpha(t)\rangle=\sum_\beta\int_{t_0}^{t'}\langle G_{\alpha,\beta}^*(t'-s)\rangle\langle f_\beta^*(s)f_\alpha(t)\rangle ds,$$

whence

$$S_F(t,t')=\int_{t_0}^{t'}G^*(t'-s)F(t,s)ds. \tag{8.20}$$

The evaluation of $\langle S_{\alpha,\alpha-\beta,\beta}(t,t')\rangle$ parallels that of $\langle H_{\alpha-\beta,\beta,\alpha}(t)\rangle$ in Sec. 4. We expand $q_\beta(t)$ and $q_\alpha^*(t')$ by iteration of the integrated form of Eq. (8.9), leaving

[19] See Appendix A.

[20] Equation (8.7) constitutes a very weak additional constraint on the ϕ's, and we anticipate that, provided $C_{2;1}=1$, it will not affect the realizability of any given set of values for the $C_{2n;p}$ when $M\to\infty$. This is verifiably so for the random coupling model: The sums $\Sigma_\beta C_{2n;p}(\alpha,\beta,\alpha-\beta)$ are unaffected $(M\to\infty)$ for either $\alpha=0$ or $\alpha\neq0$.

$\bar{q}(t)$ (which is known) explicitly in the expansion. Then we average and note the regularities imposed by the sum rule for indices and the statistical properties of the b's and the f's. The expansion for $q_\alpha^*(t')$ involves factors ϕ^*. If we express these as ϕ factors by Eq. (4.4), we are led, eventually, to the irreducible diagram expansion

$$\langle S_{\alpha,\alpha-\beta,\beta}(t,t')\rangle = M^{-1}\sum_{n=1}^{\infty}\sum_{p}^{\text{irr}} C_{2n;p}(\alpha,\alpha-\beta,\beta)\xi_{2n;p}(t,t') \quad (8.21)$$

$$(\alpha,\beta\neq 0,\ |\alpha|\neq|\beta|\neq|\alpha-\beta|),$$

where the $\xi_{2n;p}(t,t')$ are independent of α and β. From this we obtain[21]

$$S(t,t')=\sum_{n=1}^{\infty}\sum_{p}^{\text{irr}} C_{2n;p}\xi_{2n;p}(t,t'). \quad (8.22)$$

The $\xi_{2n;p}(t,t')$ may be determined by the variational method used for the $\zeta_{2n;p}(t)$ in Sec. 4. For variations which leave the $C_{2n;p}$ unchanged, we have, in correspondence to Eq. (4.16),

$$\Delta\langle S_{\alpha,\alpha-\beta,\beta}(t,t')\rangle = M^{-1}\sum_{n}\sum_{p}^{\text{irr}} \xi_{2n;p}(t,t')\Delta C_{2n;p}(\alpha,\alpha-\beta,\beta). \quad (8.23)$$

The variation Eq. (4.17), with the notation change $\beta\rightarrow\alpha-\beta$, produces perturbation terms on the right-hand sides of the equations of motion for $q_\alpha^*(t')$ and $q_\beta(t)$. In correspondence to Eq. (4.19), we find (to order $M^{-\frac{1}{2}}$)

$$\Delta q_\alpha^*(t')=\int_{t_0}^{t'} G_{\alpha,\alpha}^*(t'-s)\times[iM^{-\frac{1}{2}}\Delta\phi_{\alpha,\alpha-\beta,\beta}^* b_{\beta-\alpha}q_\beta^*(s)]ds,$$
$$\Delta q_\beta(t)=\int_{t_0}^{t} G_{\beta,\beta}(t-s)\times[-iM^{-\frac{1}{2}}\Delta\phi_{\beta,\beta-\alpha,\alpha}b_{\beta-\alpha}q_\alpha(s)]ds. \quad (8.24)$$

Then (to order M^{-1}) we find, noting

$$\Delta\phi_{\alpha,\alpha-\beta,\beta}^*=\Delta\phi_{\beta,\beta-\alpha,\alpha},$$

$$\Delta\langle S_{\alpha,\alpha-\beta,\beta}(t,t')\rangle = M^{-1}\Delta C_{2;1}(\alpha,\alpha-\beta,\beta)\times\left[\int_{t_0}^{t'}\langle G_{\alpha,\alpha}^*(t'-s)b_{\alpha-\beta}b_{\beta-\alpha}q_\beta(t)q_\beta^*(s)\rangle ds - \int_{t_0}^{t}\langle G_{\beta,\beta}(t-s)b_{\alpha-\beta}b_{\beta-\alpha}q_\alpha^*(t')q_\alpha(s)\rangle ds\right]. \quad (8.25)$$

[21] The sums over ϕ products which occur in the present case involve Σ' rather than the unrestricted summation by which the $C_{2n;p}$ are defined in Sec. 4. This does not alter the values of the sums in the limit $M\rightarrow\infty$, however.

By using Eq. (8.14) and the sharpness of $G_{\alpha,\alpha}$ and $G_{\beta,\beta}$ to reduce the averages in the limit $M\rightarrow\infty$, we have, finally,

$$\xi_{2;1}(t,t')=\langle b^2\rangle\left[\int_{t_0}^{t'} G^*(t'-s)Q(t,s)ds - \int_{t_0}^{t} G(t-s)Q^*(t',s)ds\right]. \quad (8.26)$$

It is noteworthy that this expression depends on the driving forces only implicitly, through their effect on $Q(t,t')$.

The higher $\xi_{2n;p}(t,t')$ may be found by introducing more general variations. The result is that $\xi_{2n;p}$ consists of a sum of terms each of which involves a $(2n-1)$-fold time integration over a product of $2n-1$ factors G or G^*, one Q or Q^* factor, and n factors $\langle b^2\rangle$.

We have finally to evaluate $S_C(t,t')$. It can be shown from the iteration solution of Eq. (8.9) that $\langle b_\alpha q_\alpha^*(t')\rangle$, like $\langle Q_{\alpha,\alpha}(t,t')\rangle$, has an irreducible diagram expansion and is independent of α ($\alpha\neq 0$). From the latter fact we have

$$\langle b_\alpha q_\alpha^*(t')\rangle = M^{-1}\textstyle\sum_\beta'\langle b_\beta q_\beta^*(t')\rangle + O(M^{-1}).$$

Hence, in the limit $M\rightarrow\infty$ we obtain from Eq. (8.8) the result

$$S_C(t,t')=-\bar{q}(t)[d\bar{q}^*(t')/dt'-\bar{f}^*(t')]. \quad (8.27)$$

Let us now specialize to the random coupling model. By Eq. (5.3), we then have[20]

$$S(t,t')=\xi_{2;1}(t,t'). \quad (8.28)$$

Equations (8.15), (8.19), (8.20), (8.26), (8.27), and (8.28) now permit the determination of $Q(t,t')$.

Twice the real part of Eq. (8.15) for $t=t'$ is the equation for the rate of change of the mean intensity $Q(t,t)$ of the incoherent oscillation. The quantities

$$2\,\mathrm{Re}\{S_C(t,t)\} \quad \text{and} \quad 2\,\mathrm{Re}\{S_F(t,t)\}$$

represent contributions to $dQ(t,t)/dt$ from interaction with the coherent oscillation and incoherent driving forces respectively. From Eqs. (8.26) and (8.28) we have

$$\mathrm{Re}\{S(t,t)\}=0. \quad (8.29)$$

Thus, using Eq. (8.27), we verify the conservation of total intensity,

$$(d/dt)[Q(t,t)+\bar{q}(t)\bar{q}^*(t)]=0, \quad (8.30)$$

when all the driving forces vanish. This consistency property, and Eq. (8.29) itself, are assured in advance because our equations constitute the exact description of a model for which Eq. (4.4) holds. It is also assured that the solution $Q(t,t')$ of our model equations obeys all the realizability conditions to which covariances are subject.[22]

[22] One such condition is $|Q(t,t')|^2\leq Q(t,t)Q(t',t')$.

The simplest solution of Eq. (8.15) for the random coupling model results from taking forces which vanish except for impulses at $t=t_0$ such that $Q(t_0,t_0)=1$, $\bar{q}(t_0)=0$. Then it is easily seen from Eq. (8.26), and the property $G(t)=G^*(-t)$,[23] that Eq. (8.15) becomes identical with Eq. (5.4) (for t, $t'>t_0$) under the substitution

$$Q(t,t')=G(t-t'). \tag{8.31}$$

Thus Eq. (8.31) is the solution for random shock excitation, as is required for consistency. In general, $Q(t,t')$ and $G(t-t')$ do not have the same form.

9. NON-GAUSSIAN FREQUENCY DISTRIBUTION

We shall now describe briefly the generalizations required when the distribution of $b_{[n]}$ is non-Gaussian. The case $\langle b_{[n]}\rangle\neq 0$ can be treated by methods similar to those used for $\langle f_{[n]}\rangle\neq 0$ in Sec. 8. But it is simpler to maintain the condition $\langle b_{[n]}\rangle=0$ and instead replace Eq. (8.4) by

$$(d/dt+i\bar{\omega}+\nu)q_\alpha(t) + iM^{-\frac{1}{2}}\sum_\beta \phi_{\alpha,\beta,\alpha-\beta}b_\beta q_{\alpha-\beta}(t)=f_\alpha(t), \tag{9.1}$$

where $\bar{\omega}$ is the (real) mean frequency and we have also included a real damping factor ν. It is easy to see that this generalization implies only minor changes in our treatment if $b_{[n]}$ remains Gaussian. The factor $t^{2n}/2n!$ in the iteration series Eq. (4.14) is replaced by $G^{(0)}(*G^{(0)})^{2n}$, where

$$G^{(0)}(t)=\exp[-(i\bar{\omega}+\nu)t]. \tag{9.2}$$

However, the irreducible diagram expansions for $H(t)$ and $S(t,t')$, and the expressions for the $\zeta_{2n;p}(t)$ and the $\xi_{2n;p}(t,t')$, are unchanged in form. The effect of $\bar{\omega}$, $\nu\neq 0$ is implicitly expressed by the changed *values* of the functions G and Q which appear in these expressions. The only further changes in Secs. 2–8 are the obvious replacements

$$d/dt\rightarrow(d/dt+i\bar{\omega}+\nu) \quad\text{and}\quad \partial/\partial t\rightarrow(\partial/\partial t+i\bar{\omega}+\nu)$$

where appropriate.

Now let us consider the general (non-Gaussian) case where the $b_{[n]}$ are identically distributed (with zero mean) for all n and statistically independent for different n. It is easy to verify from Eqs. (3.1) and (3.2) that Eq. (3.8) remains valid. In place of Eq. (3.10), we find

$$\begin{aligned}\langle b_\alpha\rangle&=0,\quad \langle b_\alpha b_\beta\rangle=\delta_{\alpha+\beta}\langle b^2\rangle,\\ \langle b_\alpha b_\beta b_\gamma\rangle&=\delta_{\alpha+\beta+\gamma}M^{-\frac{1}{2}}\langle b^3\rangle,\\ \langle b_\alpha b_\beta b_\gamma b_\epsilon\rangle&=(\delta_{\alpha+\beta}\delta_{\gamma+\epsilon}+\delta_{\alpha+\gamma}\delta_{\beta+\epsilon}+\delta_{\alpha+\epsilon}\delta_{\beta+\gamma})\langle b^2\rangle^2\\ &\quad+\delta_{\alpha+\beta+\gamma+\epsilon}M^{-1}(\langle b^4\rangle-3\langle b^2\rangle^2),\\ &\quad\cdots\end{aligned} \tag{9.3}$$

In general we find ($M\rightarrow\infty$) that all moments of the b_α with indices equal and opposite in pairs depend only on $\langle b^2\rangle$ and have the same values as for a Gaussian distribution of $b_{[n]}$ with this variance. Moments for which the indices do not pair (we shall call them skew moments) have values which depend on the cumulants of the $b_{[n]}$ distribution; they tend individually to zero as $M\rightarrow\infty$.[24]

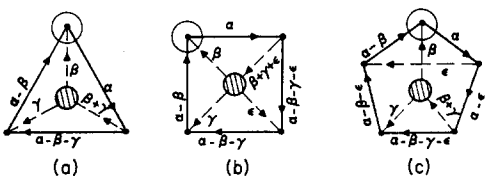

FIG. 14. Diagrams for simple non-Gaussian contributions to $G(t)$.

The presence of skew moments results in new classes of terms in Eq. (4.11) and, consequently, in Eq. (4.23). The simplest new term in Eq. (4.23) is

$$(-i)^3D_{3;1}\langle b^3\rangle G*G*G, \tag{9.4}$$

where

$$D_{3;1}=M^{-2}\sum_{\beta,\gamma}\phi_{\alpha,\beta,\alpha-\beta}\phi_{\alpha-\beta,\gamma,\alpha-\beta-\gamma}\phi_{\alpha-\beta-\gamma,-\beta-\gamma,\alpha}. \tag{9.5}$$

It may be represented by Fig. 14(a). The further terms represented by Figs. 14(b) and 14(c) are proportional to $\langle b^4\rangle-3\langle b^2\rangle^2$ and to $\langle b^2\rangle\langle b^3\rangle$, respectively.

It is possible to generalize our sequence of models so that closed equations are produced which systematically include more and more of the information expressed by the cumulants of the b distribution. We shall not attempt this here. However, it is important to note that the equations for the random coupling model are identical to those already given no matter what the (zero-mean) b distribution may be. It is clear that $D_{3;1}$ vanishes for this model ($M\rightarrow\infty$), and it can be seen that all the higher new terms in Eq. (4.23) vanish also. The statistical properties of the random coupling model thus depend only on the variance $\langle b^2\rangle$. On recalling Eq. (2.3), which is exact for the original uncoupled oscillators, we see that in certain respects the random coupling model actually will provide a better approximation for distributions of b which resemble Eq. (5.6) in form than for a Gaussian distribution.

In the physical analogs to the random oscillator which are our eventual interest, the distribution of the stochastic quantity corresponding to b may itself be determined by dynamical processes. In this case there may exist an alternative to the generalized treatment we have mentioned. It may be physically reasonable to assume Gaussian *initial conditions* for the quantities corresponding to b and q. If the dynamical equations for these quantities are then treated as a simultaneous set, the non-Gaussian diagrams will not arise in any of the relevant sequence of models. We shall give an illustration at the end of Sec. 11.

[23] This property of Eq. (5.5) is directly implied by Eq. (2.4).

[24] However, their number increases correspondingly so that those sums over individual skew moments which contribute to physical quantities remain finite in the limit.

10. PARTICLE IN A RANDOM POTENTIAL

Let the Schrödinger equation for a particle be[25]

$$(\partial/\partial t - i\nabla^2)\psi(\mathbf{x},t) = -iv(\mathbf{x})\psi(\mathbf{x},t), \qquad (10.1)$$

where $v(\mathbf{x})$ is a real potential which is statistically distributed over an infinite ensemble of realizations of the system. This problem is an exact homolog to the random oscillator with respect to treatment by stochastic models.[26] Let us consider a collection of M systems such that the individual potentials $v_{[n]}(\mathbf{x})$ are identically distributed for all n and are statistically independent for different n. Let $\psi_{[n]}(\mathbf{x},t)$ be the Schrödinger function for the nth system. Then we may define the collective quantities $\psi_\alpha(\mathbf{x},t)$ and $v_\alpha(\mathbf{x})$ in correspondence to Eq. (3.1), and consider the model equations

$$(\partial/\partial t - i\nabla^2)\psi_\alpha(\mathbf{x},t) = -iM^{-\frac{1}{2}}\sum_\beta \phi_{\alpha,\beta,\alpha-\beta} \times v_\beta(\mathbf{x})\psi_{\alpha-\beta}(\mathbf{x},t). \qquad (10.2)$$

The $\phi_{\alpha,\beta,\alpha-\beta}$ will be identical quantities for corresponding models in the present problem and the random oscillator problem.

The condition Eq. (4.4) serves to maintain hermiticity in the present case. It is easily verified from Eqs. (4.4) and (10.2) that the total probability,

$$\sum_n \int |\psi_{[n]}(\mathbf{x},t)|^2 d^3x = \sum_\alpha \int |\psi_\alpha(\mathbf{x},t)|^2 d^3x$$

and the total energy,

$$\int [-\sum_n \psi_{[n]}{}^*\nabla^2\psi_{[n]} + \sum_{n,r,s} \psi_{[n]}{}^* A_{[n,r,s]} v_{[r]}\psi_{[s]}] d^3x,$$

where $A_{[n,r,s]}$ is defined by Eq. (4.3), are conserved. However, the individual quantities $\int |\psi_{[n]}|^2 d^3x$ are not constants of motion, in general. The systems in the collection exchange particles as well as energy.

Let us now take the case where $v_{[n]}(\mathbf{x})$ has a multivariate Gaussian distribution. This implies that all odd-order moments vanish and that all even-order moments are expressible in terms of the covariance $V(\mathbf{x},\mathbf{x}') = \langle v_{[n]}(\mathbf{x})v_{[n]}(\mathbf{x}')\rangle$. In the collective representation we have

$$\begin{aligned} &\langle v_\alpha(\mathbf{x})v_\beta(\mathbf{x}')\rangle = \delta_{\alpha+\beta}V(\mathbf{x},\mathbf{x}'), \\ &\langle v_\alpha(\mathbf{x})v_\beta(\mathbf{x}')v_\gamma(\mathbf{x}'')v_\epsilon(\mathbf{x}''')\rangle \\ &\quad = \delta_{\alpha+\beta}\delta_{\gamma+\epsilon}V(\mathbf{x},\mathbf{x}')V(\mathbf{x}'',\mathbf{x}''') \\ &\qquad + \delta_{\alpha+\gamma}\delta_{\beta+\epsilon}V(\mathbf{x},\mathbf{x}'')V(\mathbf{x}',\mathbf{x}''') \\ &\qquad\quad + \delta_{\alpha+\epsilon}\delta_{\beta+\gamma}V(\mathbf{x},\mathbf{x}''')V(\mathbf{x}',\mathbf{x}''), \\ &\qquad\quad\quad \cdot\ \cdot\ \cdot\ \cdot \end{aligned} \qquad (10.3)$$

The analog of Eq. (3.8) holds, of course, whatever the distribution.

[25] We take units such that $\hbar = 1$ and $2m = 1$, where m is the particle mass.

[26] The two problems may be regarded as formally identical if b and q are interpreted as vectors in a function space and a correspondence is established between d/dt and $\partial/\partial t - i\nabla^2$.

Let us define the Green's function $G_{[n,m]}(\mathbf{x},t|\,\mathbf{x}',t')$ as the solution (for all t) of the model equation for $\psi_{[n]}(\mathbf{x},t)$ under the initial condition

$$\psi_{[r]}(\mathbf{x},t') = \delta_{r,m}\delta(\mathbf{x}-\mathbf{x}') \quad (\text{all } r),$$

and make a corresponding definition for $G_{\alpha,\gamma}(\mathbf{x},t|\,\mathbf{x}',t')$. Then, in correspondence to the analysis in Sec. 4, we find, when Eq. (4.13) is satisfied,

$$\begin{aligned} &(\partial/\partial t - i\nabla_x{}^2)G(\mathbf{x},t|\,\mathbf{x}',t') \\ &\qquad = \sum_{n=1}^{\infty}\sum_p{}^{\text{irr}} (-1)^n C_{2n;p}\zeta_{2n;p}(\mathbf{x},t|\,\mathbf{x}',t'), \qquad (10.4) \\ &\qquad G(\mathbf{x},t'|\,\mathbf{x}',t') = \delta(\mathbf{x}-\mathbf{x}'), \end{aligned}$$

where

$$\begin{aligned} \langle G_{[n,m]}(\mathbf{x},t|\,\mathbf{x}',t')\rangle &= \delta_{n,m}G(\mathbf{x},t|\,\mathbf{x}',t'), \\ \langle G_{\alpha,\gamma}(\mathbf{x},t|\,\mathbf{x}',t')\rangle &= \delta_{\alpha,\gamma}G(\mathbf{x},t|\,\mathbf{x}',t'), \end{aligned} \qquad (10.5)$$

and $\zeta_{2n;p}(\mathbf{x},t|\,\mathbf{x}',t')$ is the homolog of $\zeta_{2n;p}(t-t')$.

The functions $\zeta_{2n;p}(\mathbf{x},t|\,\mathbf{x}',t')$ may be determined by the variational method used in Sec. 4. The variation Eq. (4.17) produces, in correspondence to Eq. (4.19), the variation

$$\begin{aligned} &\Delta G_{\alpha-\beta,\alpha}(\mathbf{x},t|\,\mathbf{x}',t') \\ &\quad = \int_{t'}^{t} ds \int d^3y G_{\alpha-\beta,\alpha-\beta}(\mathbf{x},t|\,\mathbf{y},s) \\ &\qquad \times [-iM^{-\frac{1}{2}}\Delta\phi_{\alpha-\beta,-\beta,\alpha}v_{-\beta}(\mathbf{y})G_{\alpha,\alpha}(\mathbf{y},s|\,\mathbf{x}',t')], \end{aligned} \qquad (10.6)$$

and we are led, thereby, to the result

$$\begin{aligned} &\zeta_{2;1}(\mathbf{x},t|\,\mathbf{x}',t') \\ &\quad = \int_{t'}^{t} ds \int d^3y V(\mathbf{x},\mathbf{y})G(\mathbf{x},t|\,\mathbf{y},s)G(\mathbf{y},s|\,\mathbf{x}',t'), \end{aligned} \qquad (10.7)$$

which corresponds to Eq. (4.21). This result depends on the fact that $G_{\alpha,\alpha}(\mathbf{x},t|\,\mathbf{x}',t')$ is statistically sharp ($M \to \infty$), which may be demonstrated in the same way as for $G_{\alpha,\alpha}(t)$ of Sec. 4.

The result for $\zeta_{4;3}(\mathbf{x},t|\,\mathbf{x}',t')$ is

$$\begin{aligned} &\zeta_{4;3}(\mathbf{x},t|\,\mathbf{x}',t') \\ &\quad = \int_{t'}^{t} ds_1 \int_{t'}^{s_1} ds_2 \int_{t'}^{s_2} ds_3 \int\int\int d^3y_1 d^3y_2 d^3y_3 \\ &\qquad \times V(\mathbf{x},\mathbf{y}_2)V(\mathbf{y}_1,\mathbf{y}_3)G(\mathbf{x},t|\,\mathbf{y}_1,s_1)G(\mathbf{y}_1,s_1|\,\mathbf{y}_2,s_2) \\ &\qquad\quad \times G(\mathbf{y}_2,s_2|\,\mathbf{y}_3,s_3)G(\mathbf{y}_3,s_3|\,\mathbf{x}',t'). \end{aligned} \qquad (10.8)$$

The structure of expressions (10.7) and (10.8) may be represented, as in Fig. 15, by an appropriate labeling of the vertices in the diagrams for $C_{2;1}$ and $C_{4;3}$. The expressions for all the higher $\zeta_{2n;p}(\mathbf{x},t|\,\mathbf{x}',t')$ may be written down by analogy from the diagrams for the corresponding irreducible $C_{2n;p}$.

In the random coupling model, where $C_{2;1}=1$ and all the higher irreducible $C_{2n;p}$ vanish, Eq. (10.4) becomes

$$(\partial/\partial t-i\nabla_x^2)G(\mathbf{x},t|\,\mathbf{x}',t')$$

$$=-\int_{t'}^{t}ds\int d^3yV(\mathbf{x},\mathbf{y})G(\mathbf{x},t|\,\mathbf{y},s)G(\mathbf{y},s|\,\mathbf{x}',t'), \quad (10.9)$$

$$G(\mathbf{x},t'|\,\mathbf{x}',t')=\delta(\mathbf{x}-\mathbf{x}').$$

It should be pointed out that this result is independent of the assumption that the potential has a Gaussian distribution, provided that $\langle v_{[n]}(\mathbf{x})\rangle=0$ (cf. Sec. 9).[27]

We are assured that the solutions of Eq. (10.9) will exhibit certain consistency properties because this is an exact equation for a realizable model. In particular, if Eq. (10.2) is transformed into the momentum representation, it follows from a straightforward extension of the arguments given in connection with Eq. (5.7) that $G(\mathbf{x},t|\,\mathbf{x}',t')$ satisfies a basic spectral condition. The latter takes its simplest form for the homogeneous case $V(\mathbf{x},\mathbf{x}')=V(\mathbf{x}-\mathbf{x}')$, in which $G(\mathbf{x},t|\,\mathbf{x}',t')$ can depend only on $\mathbf{x}-\mathbf{x}'$ and $t-t'$. If we write

$$G_{\mathbf{k}}(t-t')=\int d^3yG(\mathbf{x},t|\,\mathbf{x}',t')\exp(-i\mathbf{k}\cdot\mathbf{y})$$

$$(\mathbf{y}=\mathbf{x}-\mathbf{x}'), \quad (10.10)$$

$$\tilde{G}_{\mathbf{k}}(\omega)=(2\pi)^{-1}\int_{-\infty}^{\infty}dsG_{\mathbf{k}}(s)\exp(i\omega s),$$

then the spectral condition is

$$\tilde{G}_{\mathbf{k}}(\omega)=|\,\tilde{G}_{\mathbf{k}}(\omega)\,|. \quad (10.11)$$

[We may note that $G_{\mathbf{k}}(t-t')$ is the diagonal response function for the amplitude in the mode $\mathbf{k}$.] Equation (10.11) implies the reciprocity relation

$$G(\mathbf{x},t|\,\mathbf{x}',t')=G^*(\mathbf{x}',t'|\,\mathbf{x},t). \quad (10.12)$$

When $V(\mathbf{x},\mathbf{x}')=V(\mathbf{x}-\mathbf{x}')$, Eq. (10.9) has the transform

$$(\partial/\partial t+ik^2)G_{\mathbf{k}}(t)=-\int^{t}ds\int d^3k'V_{\mathbf{k}-\mathbf{k}'}G_{\mathbf{k}'}(t-s)G_{\mathbf{k}}(s),$$

$$G_{\mathbf{k}}(0)=1, \quad (10.13)$$

where

$$V_{\mathbf{k}}=(2\pi)^{-3}\int d^3yV(\mathbf{y})\exp(-i\mathbf{k}\cdot\mathbf{y}).$$

It is possible to solve Eq. (10.13) easily for very high k (the WKBJ limit). This is of particular interest because it is well known that the perturbation approach breaks down in this limit. Let us take k sufficiently high that $V_{\mathbf{k}-\mathbf{k}'}\approx 0$, unless $|\mathbf{k}-\mathbf{k}'|\ll k$. Then it is plausible that we may replace $G_{\mathbf{k}'}(t-s)$ by $G_{\mathbf{k}}(t-s)$ in Eq. (10.13) and

[27] When the latter condition is not fulfilled, an additional term $i\bar{v}(\mathbf{x})G(\mathbf{x},t|\,\mathbf{x}',t')$ appears on the left-hand side of Eq. (10.4), where $\bar{v}(\mathbf{x})$ is the mean potential, and $V(\mathbf{x},\mathbf{y})$ then is defined in terms of the zero-mean part of the potential.

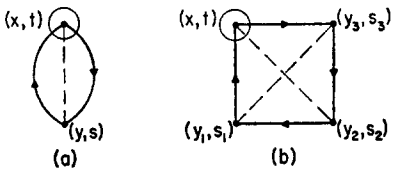

FIG. 15. Diagrams for $\zeta_{2;1}(\mathbf{x},t|\,\mathbf{x}',t')$ and $\zeta_{4;3}(\mathbf{x},t|\,\mathbf{x}',t')$.

thereby obtain[28]

$$(\partial/\partial t+ik^2)G_{\mathbf{k}}(t)=-\langle v^2\rangle\int_0^t G_{\mathbf{k}}(t-s)G_{\mathbf{k}}(s)ds,$$

$$G_{\mathbf{k}}(0)=1, \quad (10.14)$$

where

$$\langle v^2\rangle=V(0)=\int V_{\mathbf{k}}d^3k.$$

Equation (10.14) becomes identical with Eq. (5.4) under the transformation

$$G_{\mathbf{k}}(t)\rightarrow\exp(-ik^2t)G(t), \quad \langle v^2\rangle\rightarrow\langle b^2\rangle.$$

Consequently, we have

$$\tilde{G}_{\mathbf{k}}(\omega)=(\pi v_*)^{-1}\left[1-\left(\frac{\omega-k^2}{2v_*}\right)^2\right]^{\frac{1}{2}} \quad (|\omega-k^2|\leq 2v_*),$$

$$=0 \quad (|\omega-k^2|>2v_*), \quad (10.15)$$

where $v_*=\langle v^2\rangle^{\frac{1}{2}}$. This correspondence between the WKBJ limit and the random oscillator is not confined to the random coupling model. If Eq. (10.4) is written in the k representation in this limit, and the previous transformation is made, the resulting equation is identical with Eq. (4.23). A particular consequence is that the WKBJ solution to the true problem (all ϕ's=1) is

$$\tilde{G}_{\mathbf{k}}(\omega)=(2\pi\langle v^2\rangle)^{-\frac{1}{2}}\exp[-\tfrac{1}{2}(\omega-k^2)^2/\langle v^2\rangle], \quad (10.16)$$

in correspondence to Eq. (2.7). This result states that for sharp kinetic energy (sharp k) the total energy distribution follows the Gaussian potential energy distribution. Considered as an approximation to Eq. (10.16), the random coupling result (10.15) exhibits the qualitative physical fact that sharp momentum states are not sharp energy states. The quantitative form of Eq. (10.15) suggests that the random coupling model may represent a better approximation to the true problem if the true potential distribution has a clipped rather than a Gaussian form (cf. Sec. 9). It should be noted that the cumulant-discard approximation scheme, when applied in the WKBJ limit, yields expressions for $\exp(ik^2t)G_{\mathbf{k}}(t)$ which are identical in form to Eq. (2.13). This implies discrete spectra $\tilde{G}_{\mathbf{k}}(\omega)$, which is unphysical compared to the random coupling result.

The general correspondence between the WKBJ limit and the random oscillator includes, of course, the second stochastic model, discussed in Sec. 7. The WKBJ

[28] This procedure can be justified *a posteriori*.

results for the two stochastic models and for the true problem in the Gaussian case are given by Fig. 13, if the horizontal and vertical axes are relabeled $(\omega-k^2)/v_*$ and $\pi v_* \tilde{G}_k(\omega)$, respectively. Away from the WKBJ limit, the analysis of the second model is considerably more difficult than for the random oscillator, although the same in principle. The equations are not reducible to algebraic form, and the analogs to the inverses $[\mathbf{G}(p)]^{-1}$ and $\langle b^2\rangle^{-1}$, which appeared in Sec. 7, must be defined by integral equations.

Let us assume that the Schrödinger fields are switched on at $t=t_0$ in such a way that the $\psi_{[n]}(\mathbf{x},t_0)$ are statistically independent and identically distributed for all n and statistically independent of $v_{[r]}(\mathbf{x})$ for all r. Let

$$\psi_{[n]}(\mathbf{x},t)=\bar{\psi}(\mathbf{x},t)+\psi_{[n]}'(\mathbf{x},t), \qquad \bar{\psi}(\mathbf{x},t)=\langle\psi_{[n]}(\mathbf{x},t)\rangle. \tag{10.17}$$

We shall call $\bar{\psi}(\mathbf{x},t)$ the coherent wave and $\psi_{[n]}'(\mathbf{x},t)$ the incoherent wave. The evolution of the coherent amplitude and the incoherent covariance may be determined by direct correspondence to the analysis in Sec. 8.

Noting that our switch-on is equivalent to the action of impulsive sources $f_{[n]}(\mathbf{x},t)=\psi_{[n]}(\mathbf{x},t_0)\delta(t-t_0)$, we have, in correspondence to Eq. (8.11),

$$\bar{\psi}(\mathbf{x},t)=\int G(\mathbf{x},t\,|\,\mathbf{y},t_0)\bar{\psi}(\mathbf{y},t_0)d^3y. \tag{10.18}$$

When the potential is statistically homogeneous, Eq. (10.18) has the transform

$$\bar{\psi}_{\mathbf{k}}(t)=G_{\mathbf{k}}(t-t_0)\bar{\psi}_{\mathbf{k}}(t_0), \tag{10.19}$$

where

$$\bar{\psi}_{\mathbf{k}}(t)=(2\pi)^{-3}\int\bar{\psi}(\mathbf{x},t)\,\exp(-i\mathbf{k}\cdot\mathbf{x})d^3x.$$

In this case the various momentum modes of the coherent wave evolve independently. As our WKBJ limit results illustrate, $G_{\mathbf{k}}(t)$ has a continuous spectrum and, therefore, vanishes as $t\to\infty$. Consequently, the coherent wave eventually is extinguished by its interaction with the random potential.

In direct correspondence to the results obtained in Sec. 8, we have

$$\langle\psi_{[n]}'(\mathbf{x},t)\psi_{[m]}'^*(\mathbf{x}',t')\rangle=\delta_{n,m}\Psi(\mathbf{x},t;\,\mathbf{x}',t'), \qquad \langle\psi_\alpha(\mathbf{x},t)\psi_\gamma^*(\mathbf{x}',t')\rangle=\delta_{\alpha,\gamma}\Psi(\mathbf{x},t;\,\mathbf{x}',t') \quad (\alpha\neq 0), \tag{10.20}$$

where $\Psi(\mathbf{x},t;\,\mathbf{x}',t')$ has the symmetry property

$$\Psi(\mathbf{x},t;\,\mathbf{x}',t')=\Psi^*(\mathbf{x}',t';\,\mathbf{x},t), \tag{10.21}$$

and obeys

$$(\partial/\partial t-i\nabla_x^2)\Psi(\mathbf{x},t;\,\mathbf{x}',t')=S(\mathbf{x},t;\,\mathbf{x}',t')+S_C(\mathbf{x},t;\,\mathbf{x}',t'), \tag{10.22}$$

with

$$S(\mathbf{x},t;\,\mathbf{x}',t')=\sum_{n=1}^{n}\sum_{p}^{\text{irr}}C_{2n;p}\xi_{2n;p}(\mathbf{x},t;\,\mathbf{x}',t'), \tag{10.23}$$

and

$$S_C(\mathbf{x},t;\,\mathbf{x}',t')=-\bar{\psi}(\mathbf{x},t)(\partial/\partial t'+i\nabla_{x'}^2)\bar{\psi}^*(\mathbf{x}',t'). \tag{10.24}$$

There is no term corresponding to $S_P(t,t')$ because we have not admitted sources for $t>t_0$.

The functions $\xi_{2n;p}(\mathbf{x},t;\,\mathbf{x}',t')$, which are homologous to the $\xi_{2n;p}(t,t')$ in Eq. (8.22), may be determined by employing our variational procedure and noting the statistical property

$$\langle v_\beta(\mathbf{x}_1)v_{-\beta}(\mathbf{x}_1')\cdots v_\mu(\mathbf{x}_r)v_{-\mu}(\mathbf{x}_r')\psi_\alpha(\mathbf{y},t)\psi_\alpha^*(\mathbf{y}',t')\rangle = V(\mathbf{x}_1,\mathbf{x}_1')\cdots V(\mathbf{x}_r,\mathbf{x}_r')\Psi(\mathbf{y},t;\,\mathbf{y}',t')+O(M^{-1}) \quad (\alpha\neq 0,\quad |\alpha|=|\beta|\neq\cdots\neq|\mu|), \tag{10.25}$$

which corresponds to Eq. (8.14). (Here $\mathbf{x}_1$, $\mathbf{x}_1'$, etc., are arbitrary position vectors.) In particular, we find

$$\xi_{2;1}(\mathbf{x},t;\,\mathbf{x}',t')=\int d^3yV(\mathbf{x},\mathbf{y})\Big[\int_{t_0}^{t'}dsG^*(\mathbf{x}',t'\,|\,\mathbf{y},s)\Psi(\mathbf{x},t;\,\mathbf{y},s) -\int_{t_0}^{t}dsG(\mathbf{x},t\,|\,\mathbf{y},s)\Psi^*(\mathbf{x}',t';\,\mathbf{y},s)\Big]. \tag{10.26}$$

For the random coupling model,

$$S(\mathbf{x},t;\,\mathbf{x}',t')=\xi_{2;1}(\mathbf{x},t;\,\mathbf{x}',t'), \tag{10.27}$$

and we have a closed set of equations which determine $\Psi(\mathbf{x},t;\,\mathbf{x}',t')$ when the initial functions $\Psi(\mathbf{x},t_0;\,\mathbf{x}',t_0)$ and $\bar{\psi}(\mathbf{x},t_0)$ are given. As was the case for $G(\mathbf{x},t\,|\,\mathbf{x}',t')$, certain important consistency properties necessarily are exhibited by the solution $\Psi(\mathbf{x},t;\,\mathbf{x}',t')$ for any realizable model. In particular, we are assured that $\Psi(\mathbf{x},t;\,\mathbf{x}',t')$ satisfies all the realizability conditions to which a covariance is subject. In the homogeneous case, where the spatial dependence of $\Psi(\mathbf{x},t;\,\mathbf{x}',t')$ involves only $\mathbf{x}-\mathbf{x}'$, we must have

$$\Psi_{\mathbf{k}}(t,t)=|\Psi_{\mathbf{k}}(t,t)|, \tag{10.28}$$

where

$$\Psi_{\mathbf{k}}(t,t')=(2\pi)^{-3}\int\Psi(\mathbf{x},t;\,\mathbf{x}',t')\,\exp(-i\mathbf{k}\cdot\mathbf{y})d^3y \qquad (\mathbf{y}=\mathbf{x}-\mathbf{x}').$$

When $t_0\to-\infty$ and a statistically stationary state has been set up, so that $\Psi_{\mathbf{k}}(t,t')=\Psi_{\mathbf{k}}(t-t')$, we have, further,

$$\tilde{\Psi}_{\mathbf{k}}(\omega)=|\tilde{\Psi}_{\mathbf{k}}(\omega)|, \tag{10.29}$$

where

$$\tilde{\Psi}_{\mathbf{k}}(\omega)=(2\pi)^{-1}\int_{-\infty}^{\infty}\Psi_{\mathbf{k}}(t)\,\exp(i\omega t)dt.$$

In contrast, cumulant-discard approximations similar to those of Sec. 2 may lead, in the present problem, to *negative* occupation probabilities, $\Psi_{\mathbf{k}}(t,t)<0$, for physically admissible initial conditions. Such behavior is easily verified in simpler, but analogous, dynamical systems.

Twice the real part of Eq. (10.22) for $\mathbf{x}',t'=\mathbf{x},t$ represents the continuity equation for the ensemble mean of the quantum-mechanical probability of finding a particle. The left-hand side is the quantum-mechanical equivalent of the substantial derivative of the mean probability density $\Psi(\mathbf{x},t;\mathbf{x},t)$ in the incoherent wave. The corresponding quantity for the coherent wave is $-2\,\mathrm{Re}\{S_C(\mathbf{x},t;\mathbf{x},t)\}$. It is clear from Eqs. (10.27) and (10.26) that $\mathrm{Re}\{S(\mathbf{x},t;\mathbf{x},t)\}$ vanishes. Consequently, the continuity equation simply states that a particle enters the incoherent wave as it leaves the coherent wave.

The vanishing of $\mathrm{Re}\{S(\mathbf{x},t;\mathbf{x},t)\}$ expresses the fact that the direct effect of the potential on the particles is to change their momentum rather than their position. To illustrate this, let us take $\bar{\psi}(\mathbf{x},t)=0$ and assume that the potential and the incoherent wave are statistically homogeneous. Then from the Fourier transforms of Eqs. (10.22), (10.27), and (10.26), we obtain

$$d\Psi_{\mathbf{k}}(t,t)/dt$$

$$=2\,\mathrm{Re}\int_{t_0}^{t}ds\int d^3k'V_{\mathbf{k}-\mathbf{k}'}[G_{\mathbf{k}}(s-t)\Psi_{\mathbf{k}'}(t,s)-G_{\mathbf{k}'}(t-s)\Psi_{\mathbf{k}}(s,t)], \quad (10.30)$$

after noting Eqs. (10.12) and (10.21). The quantity $\Psi_{\mathbf{k}}(t,t)$ is the mean probability density for finding a particle with momentum $\mathbf{k}$. The right side of Eq. (10.30), therefore, is the rate of transfer of particles to this momentum from all other momenta $\mathbf{k}'$. It is easily verified from Eq. (10.30) that $\int\Psi_{\mathbf{k}}(t,t)d^3k$ is a constant of motion.

Suppose that the fields have been switched on at $t_0=-\infty$ in such fashion that a stationary state exists at time t. By using Eqs. (10.11) and (10.29), the right-hand side of Eq. (10.30) may be rewritten so that we have

$$0=d\Psi_{\mathbf{k}}(t,t)/dt$$

$$=\int_{-\infty}^{\infty}d\omega\int d^3k'V_{\mathbf{k}-\mathbf{k}'}[\tilde{G}_{\mathbf{k}}(\omega)\tilde{\Psi}_{\mathbf{k}'}(\omega)-\tilde{G}_{\mathbf{k}'}(\omega)\tilde{\Psi}_{\mathbf{k}}(\omega)]. \quad (10.31)$$

We note that the right-hand side of Eq. (10.31) is the difference of two terms each of which is positive.[29] The first represents an input of particles to mode $\mathbf{k}$ from other modes $\mathbf{k}'$ and the second represents an output to these other modes. If the excitation of mode $\mathbf{k}$ only were to be slowly increased by some outside agency, it is clear that the output term would increase in magnitude while the input term would be initially unaffected. Thus, the random coupling model exhibits a plausible tendency to restore statistical equilibrium.

It will be noted that Eq. (10.31) is satisfied in general if

$$\tilde{\Psi}_{\mathbf{k}}(\omega)=f(\omega)\tilde{G}_{\mathbf{k}}(\omega), \quad (10.32)$$

where $f(\omega)$ is a function independent of $\mathbf{k}$. Now it can be seen from their definitions that $\tilde{G}_{\mathbf{k}}(\omega)$ is proportional to the density of eigenstates of energy ω available to a particle of momentum $\mathbf{k}$, while $\tilde{\Psi}_{\mathbf{k}}(\omega)$ is proportional to the occupation of such states by particles of this momentum. Thus Eq. (10.32) has the usual form of a single-particle equilibrium distribution law if $f(\omega)$ is a function of ω/θ (θ= temperature) appropriate to the statistics of the particle.[30] In a later paper, we shall deduce distribution laws of this form directly from a condition of statistical equilibrium under small perturbations in the coupling among systems in a collection, without appealing to probability distributions in the space of the eigenstates (such as the grand canonical distribution).

11. TURBULENCE DYNAMICS

The problem of turbulence dynamics serves to illustrate the application of our methods to equations of motion which are nonlinear in the dynamic variables. In order to keep the formalism as simple as possible, we shall work here with the one-dimensional scalar analog to the Navier-Stokes equation proposed by Burgers.[31] The treatment of the Navier-Stokes equation for an incompressible fluid, which we shall discuss briefly, does not differ in essentials.

Burgers' equation is

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)u(x,t)=-u(x,t)\frac{\partial u(x,t)}{\partial x}=-\frac{1}{2}\frac{\partial}{\partial x}[u(x,t)]^2. \quad (11.1)$$

The function $u(x,t)$ may be interpreted as the velocity of an infinitely compressible fluid, of constant kinematic viscosity ν, executing one-dimensional motion. If $\nu=0$, the quantities

$$\int_{-\infty}^{\infty}u(x,t)dx, \quad \tfrac{1}{2}\int_{-\infty}^{\infty}[u(x,t)]^2dx$$

are both constants of motion. We shall call them "momentum" and "energy," respectively. [This is not their accurate meaning, however, on the basis of the interpretation just suggested for $u(x,t)$.]

If an infinitesimal forcing term $\delta f(x,t)$ is added to the right side of Eq. (11.1) for $t>t_0$, the response is

$$\delta u(x,t)=\int_{t_0}^{t}ds\int_{-\infty}^{\infty}dyG_{[\,]}(x,t|y,s)\delta f(y,s),$$

where the infinitesimal Green's function $G_{[\,]}(x,t|x',t')$

[29] $V_{\mathbf{k}}$ necessarily is real and nonnegative.

[30] We may note that $\int d^3kG_{\mathbf{k}}(-i\theta^{-1})=G(\mathbf{x},-i\theta^{-1}|\mathbf{x},0)$ is the mean one-particle partition function per unit volume.

[31] J. M. Burgers, Advances in Appl. Mech. 1, 171 (1948).

obeys

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)G_{[\ ]}(x,t|x',t') = -\frac{\partial}{\partial x}[u(x,t)G_{[\ ]}(x,t|x',t')], \tag{11.2}$$

$$G_{[\ ]}(x,t'|x',t')=\delta(x-x').$$

In correspondence to the procedure followed in Secs. 4, 8, and 10, let us take a collection of systems with velocity fields $u_{[n]}(x,t)$ and Green's functions

$$G_{[n,m]}(x,t|x',t'),$$

pass to the collective representation, and consider, instead of Eqs. (11.1) and (11.2), model equations of the form

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)u_\alpha(x,t) = -\tfrac{1}{2}M^{-\frac{1}{2}}\sum_\beta \phi_{\alpha,\beta,\alpha-\beta}\frac{\partial}{\partial x}[u_\beta(x,t)u_{\alpha-\beta}(x,t)], \tag{11.3}$$

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)G_{\alpha,\gamma}(x,t|x',t') = -M^{-\frac{1}{2}}\sum_\beta \phi_{\alpha,\beta,\alpha-\beta}\frac{\partial}{\partial x}[u_\beta(x,t)G_{\alpha-\beta,\gamma}(x,t|x',t')],$$

$$G_{\alpha,\gamma}(x,t'|x',t')=\delta_{\alpha,\gamma}\delta(x-x'). \tag{11.4}$$

As before, the ϕ's are independent of x and t and the same for all ensemble-realizations of the collection.

We shall impose upon the ϕ's the three conditions

$$\phi_{\alpha,\beta,\alpha-\beta}=\phi_{\alpha,\alpha-\beta,\beta},\quad \phi_{-\alpha,-\beta,-\alpha+\beta}=\phi_{\alpha,\beta,\alpha-\beta}{}^*,\quad \phi_{\alpha-\beta,-\beta,\alpha}=\phi_{\alpha,\beta,\alpha-\beta}{}^*. \tag{11.5}$$

The first is a symmetry convention. It does not restrict the dynamics.[32] The second insures that Eq. (11.3) preserves the property

$$u_\alpha(x,t)=u_{-\alpha}{}^*(x,t)$$

and, therefore, the reality of the $u_{[n]}(x,t)$. The third is identical with Eq. (4.4). It insures that

$$\tfrac{1}{2}\sum_n\int_{-\infty}^{\infty}[u_{[n]}(x,t)]^2dx=\tfrac{1}{2}\sum_\alpha\int_{-\infty}^{\infty}|u_\alpha(x,t)|^2dx$$

FIG. 16. Vertex representations for the turbulence problem.

[32] We have, in fact, assumed this condition in writing Eq. (11.4).

is a constant of motion, if $\nu=0$. The property

$$\frac{d}{dt}\int_{-\infty}^{\infty}u_{[n]}(x,t)dx=0$$

follows from Eq. (11.3) for any values of the ϕ's, provided the $u_{[n]}(x,t)$ vanish at $x=\infty$. In correspondence to Eq. (8.7) we shall also require

$$\phi_{\mu,\lambda,\sigma}=1 \quad (\mu,\lambda \text{ or } \sigma=0). \tag{11.6}$$

The additional conditions which the ϕ's now satisfy imply only minor modifications in the diagrammatic representation introduced in Sec. 4. Let us associate with $\phi_{\mu,\lambda,\sigma}$ and $\phi_{\mu,\lambda,\sigma}{}^*$ the vertices shown in Figs. 16(a) and 16(b), respectively. Then the rules for associating diagrams with $C_{2n;p}(\alpha,\beta,\alpha-\beta)$ and $C_{2n;p}$ are identical with those given in Sec. 4, if dashed lines are replaced by solid lines everywhere.[33] We shall assume hereafter that Eq. (4.13) is satisfied.

Let us take

$$u_{[n]}(x,t_0)=\bar{u}(x,t_0)+u_{[n]}{}'(x,t_0), \tag{11.7}$$

where the initial values $u_{[n]}{}'(x,t_0)$ are identically distributed, with zero mean, for each n and statistically independent for different n. In correspondence to Eq. (3.8), it then follows that the moments of the $u_\alpha(x,t_0)$ vanish unless the sum of indices is zero. Now suppose that Eq. (11.3) is solved by iteration. From this property of the initial value moments, and the combination rule for indices in Eq. (11.3), we find

$$\langle u_\alpha(x,t)u_\beta(x',t')\cdots\rangle=0 \quad (\alpha+\beta+\cdots\neq 0). \tag{11.8}$$

Similarly, the iteration solution of Eq. (11.4) yields

$$\langle G_{\alpha,\gamma}(x,t|x',t')\rangle=0 \quad (\alpha\neq\gamma). \tag{11.9}$$

It follows immediately from Eq. (11.8) that

$$\langle u_{[n]}(x,t)\rangle=\langle M^{-\frac{1}{2}}u_0(x,t)\rangle$$

for all n. In correspondence to the similar result cited in Sec. 8, it can be shown that $M^{-\frac{1}{2}}u_0(x,t)$ is a sharp quantity ($M\to\infty$). Let us write

$$u_{[n]}(x,t)=\bar{u}(x,t)+u_{[n]}{}'(x,t),\quad \bar{u}(x,t)=\langle u_{[n]}(x,t)\rangle. \tag{11.10}$$

We shall call $\bar{u}(x,t)$ and $u_{[n]}{}'(x,t)$ the mean and fluctuating fields, respectively. By identifying $M^{-\frac{1}{2}}u_0(x,t)$ with $\bar{u}(x,t)$ in the limit $M\to\infty$, and noting Eq. (11.6), we may now rewrite Eqs. (11.3) and (11.4) in the form

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)\bar{u}(x,t)+\bar{u}(x,t)\frac{\partial\bar{u}(x,t)}{\partial x} = -\tfrac{1}{2}M^{-1}{\sum_\alpha}'\frac{\partial}{\partial x}\langle u_\alpha(x,t)u_{-\alpha}(x,t)\rangle, \tag{11.11}$$

[33] The additional symmetry properties expressed by Eq. (11.5) result in an ambiguity in the formal expressions for the $C_{2n;p}$ given by the rules in Sec. 4. There is, however, no ambiguity in value.

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)u_\alpha(x,t)+\frac{\partial}{\partial x}[\bar{u}(x,t)u_\alpha(x,t)]$$

$$=-\tfrac{1}{2}M^{-1}\sum_\beta{}''\,\phi_{\alpha,\beta,\alpha-\beta}\frac{\partial}{\partial x}[u_\beta(x,t)u_{\alpha-\beta}(x,t)]$$

$$(\alpha\neq 0), \quad (11.12)$$

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)G_{\alpha,\gamma}(x,t|x',t')+\frac{\partial}{\partial x}[\bar{u}(x,t)G_{\alpha,\gamma}(x,t|x',t')]$$

$$=-M^{-\frac{1}{2}}\sum_\beta{}'\,\phi_{\alpha,\beta,\alpha-\beta}\frac{\partial}{\partial x}[u_\beta(x,t)G_{\alpha-\beta,\gamma}(x,t|x',t')],$$

$$G_{\alpha,\gamma}(x,t'|x',t')=\delta_{\alpha,\gamma}\delta(x-x'), \quad (11.13)$$

where $\sum_\beta{}'$ implies that $\beta=0$ is to be omitted and $\sum_\beta{}''$ implies that both $\beta=0$ and $\alpha-\beta=0$ are to be omitted. It should be noted that Eq. (11.13) has the same form for $\alpha\neq 0$ and $\alpha=0$. Equations (11.11) and (11.12) are coupled equations which determine the evolution of the mean and fluctuating fields.

Now let us assume that the distribution of the initial values $u_{[n]}'(x,t_0)$ is multivariate Gaussian. It can then be shown from the iteration solutions of Eqs. (11.12) and (11.13), using arguments similar to those in Secs. 4 and 8, that $\langle u_\alpha(x,t)u_{-\alpha}(x',t')\rangle$ is independent of α ($\alpha\neq 0$) and that $\langle G_{\alpha,\alpha}(x,t|x',t')\rangle$ is independent of α (all α). Then it follows from Eqs. (11.8) and (11.9) that

$$\begin{aligned}\langle u_{[n]}'(x,t)u_{[m]}'(x',t')\rangle&=\delta_{n,m}U(x,t;x',t'),\\ U(x,t;x',t')&=\langle u_\alpha(x,t)u_{-\alpha}(x',t')\rangle \quad (\alpha\neq 0),\\ \langle G_{[n,m]}(x,t|x',t')\rangle&=\delta_{n,m}G(x,t|x',t'),\\ G(x,t|x',t')&=\langle G_{\alpha,\alpha}(x,t|x',t')\rangle.\end{aligned} \quad (11.14)$$

In correspondence to our previous results, $G_{\alpha,\alpha}(x,t|x',t')$ is statistically sharp ($M\to\infty$), and the covariances satisfy

$$\begin{aligned}&\langle u_\alpha(x,t)u_{-\alpha}(x',t')u_\beta(y,s)u_{-\beta}(y',s')\cdots\rangle\\ &\quad=U(x,t;x',t')U(y,s;y',s')\cdots+O(M^{-1}) \quad (11.15)\\ &\qquad(\alpha,\beta,\cdots\neq 0,\ |\alpha|\neq|\beta|\neq\cdots)\end{aligned}$$

[cf. Eq. (8.14)]. It follows from Eq. (11.14) that $U(x,t;x',t')$ has the symmetry property

$$U(x,t;x',t')=U(x',t';x,t). \quad (11.16)$$

From Eqs. (11.12) and (11.13) we find that $U(x,t;x',t')$ and $G(x,t|x',t')$ satisfy equations of the form

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)U(x,t;x',t')+\frac{\partial}{\partial x}[\bar{u}(x,t)U(x,t;x',t')]$$

$$=S(x,t;x',t'), \quad (11.17)$$

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)G(x,t|x',t')+\frac{\partial}{\partial x}[\bar{u}(x,t)G(x,t|x',t')]$$

$$=H(x,t|x',t'), \quad (11.18)$$

$$G(x,t'|x',t')=\delta(x-x'),$$

where it follows from the iteration solutions, with Gaussian $u_{[n]}'(x,t_0)$, that $S(x,t;x',t')$ and $H(x,t|x',t')$ have the forms

$$S(x,t;x',t')=\sum_n\sum_p^{\text{irr}}C_{2n;p}\xi_{2n;p}(x,t;x',t'), \quad (11.19)$$

and

$$H(x,t|x',t')=\sum_n\sum_p^{\text{irr}}C_{2n;p}\zeta_{2n;p}(x,t|x',t').^{21} \quad (11.20)$$

To complete the set of equations, we may rewrite Eq. (11.11) in the form

$$\left(\frac{\partial}{\partial t}-\nu\frac{\partial^2}{\partial x^2}\right)\bar{u}(x,t)+\bar{u}(x,t)\frac{\partial\bar{u}(x,t)}{\partial x}$$

$$=-\frac{1}{2}\frac{\partial}{\partial x}U(x,t;x,t). \quad (11.21)$$

Equation (11.21) is the balance equation for mean "momentum" density and Eq. (11.17) for $x',t'=x,t$ is the balance equation for the mean "energy" density in the fluctuating field.

The functions $\xi_{2n;p}(x,t;x',t')$ and $\zeta_{2n;p}(x,t|x',t')$ may be determined by the variational procedure of Sec. 4, using Eq. (11.15) and the statistical sharpness of $G_{\alpha,\alpha}(x,t|x',t')$. The results for $\xi_{2;1}(x,t;x',t')$ and $\zeta_{2;1}(x,t|x',t')$ are

$$\begin{aligned}&\xi_{2;1}(x,t;x',t')\\ &=-\frac{1}{2}\frac{\partial}{\partial x}\int_{t_0}^{t'}ds\int_{-\infty}^{\infty}dyG(x',t'|y,s)\frac{\partial}{\partial y}[U(x,t;y,s)]^2\\ &\quad+\frac{\partial}{\partial x}\int_{t_0}^{t}ds\int_{-\infty}^{\infty}dyG(x,t|y,s)\\ &\qquad\times\frac{\partial}{\partial y}[U(x,t;y,s)U(x',t';y,s)],\end{aligned} \quad (11.22)$$

$$\zeta_{2;1}(x,t|x',t')=\frac{\partial}{\partial x}\int_{t_0}^{t}ds\int_{-\infty}^{\infty}dyG(x,t|y,s)$$

$$\times\frac{\partial}{\partial y}[U(x,t;y,s)G(y,s|x',t')]. \quad (11.23)$$

In general $\xi_{2n;p}(x,t;x',t')$ consists of a sum of terms each of which involves a $(2n-1)$-fold space-time integration over a product of $2n-1$ factors G and $n+1$

factors U. The terms comprising $\zeta_{2n;p}(x,t|x',t')$ each involve a $(2n-1)$-fold integration over a product of $2n$ factors G and n factors U.

We shall illustrate the variational procedure in the present case by outlining the analysis for $\xi_{2;1}(x,t;x',t')$. In correspondence to Eq. (8.16), we may write, for the present problem,

$$S(x,t;x',t')=\sum_\beta{}''\langle S_{\alpha,\beta,\alpha-\beta}(x,t;x',t')\rangle \quad (\alpha\neq 0),$$

$$S_{\alpha,\beta,\alpha-\beta}(x,t;x',t')=-\tfrac{1}{2}M^{-\frac{1}{2}}\phi_{\alpha,\beta,\alpha-\beta}\frac{\partial}{\partial x}[u_\beta(x,t) \times u_{\alpha-\beta}(x,t)u_{-\alpha}(x',t')]. \tag{11.24}$$

Then the iteration solution yields

$$\langle S_{\alpha,\beta,\alpha-\beta}(x,t;x',t')\rangle = M^{-1}\sum_{n=1}^{\infty}\sum_{p}^{\text{irr}} C_{2n;p}(\alpha,\beta,\alpha-\beta)\xi_{2n;p}(x,t;x',t') \tag{11.25}$$

$$(\alpha,\beta,\alpha-\beta\neq 0, \quad |\alpha|\neq|\beta|\neq|\alpha-\beta|),$$

which corresponds to Eq. (8.21), and is the basis for Eq. (11.19). Now consider the variation Eq. (4.17). By using Eq. (11.5) several times, we find

$$\Delta\phi_{\alpha-\beta,-\beta,\alpha}=\Delta\phi_{\alpha-\beta,\alpha,-\beta}=\Delta\phi_{\beta,-\alpha+\beta,\alpha} =\Delta\phi_{\beta,\alpha,-\alpha+\beta}=\Delta\phi_{-\alpha,-\beta,-\alpha+\beta}=\Delta\phi_{-\alpha,-\alpha+\beta,-\beta}.$$

Hence, recalling Eq. (11.3), we find

$$\Delta u_\beta(x,t)=\int_{t_0}^{t}ds\int_{-\infty}^{\infty}dy G_{\beta,\beta}(x,t|y,s) \times\left\{-M^{-\frac{1}{2}}\Delta\phi_{\beta,\alpha,-\alpha+\beta}\frac{\partial}{\partial y}[u_\alpha(y,s)u_{-\alpha+\beta}(y,s)]\right\}, \tag{11.26}$$

to order $M^{-\frac{1}{2}}$, with expressions of the same type for $\Delta u_{\alpha-\beta}(x,t)$ and $\Delta u_{-\alpha}(x',t')$.[34] These results correspond to Eq. (8.24). It is important to note that the perturbation terms are $O(M^{-\frac{1}{2}})$, so that the infinitesimal Green's functions correctly may be used to find the induced variations. Now we may express

$$\Delta\langle S_{\alpha,\beta,\alpha-\beta}(x,t;x',t')\rangle$$

to $O(M^{-1})$ in correspondence to Eq. (8.25), reduce the averages by using Eq. (11.15) and the sharpness of the $G_{\alpha,\alpha}$, and appeal to the analog of Eq. (8.23). Thereby, we obtain the result Eq. (11.22).

The random coupling model for the present problem is obtained by assigning the ϕ's as in Sec. 5, but with the additional constraints Eqs. (11.5) and (11.6). It is clear that these constraints do not affect Eq. (5.3) in the limit $M\to\infty$. Hence, we have

$$S(x,t;x',t')=\xi_{2;1}(x,t;x',t'), \quad H(x,t|x',t')=\zeta_{2;1}(x,t|x',t') \tag{11.27}$$

for this model. These relations, together with Eqs. (11.16)–(11.18) and Eqs. (11.21)–(11.23), form a closed set which determine $\bar{u}(x,t)$, $U(x,t;x',t')$, and $G(x,t|x',t')$ in terms of the initial functions $\bar{u}(x,t_0)$ and $U(x,t_0;x',t_0)$.

The most essential difference between the present equations and the analogous ones for the random potential problem given in Sec. 10 is that $G(x,t|x',t')$ is not independent of $U(x,t;x',t')$ and $\bar{u}(x,t)$ in the present case; all three quantities now must be determined simultaneously. A further consequence of the nonlinearity is that $\bar{u}(x,t)$ does not have an expression analogous to Eq. (10.18). The Green's function $G(x,t|x',t')$ can only describe the propagation of infinitesimal disturbances $\delta\bar{u}(x',t')$. In general, $\bar{u}(x,t)\neq 0$ even if $\bar{u}(x,t_0)=0$ everywhere.

The Navier-Stokes equation for the velocity $\mathbf{u}(\mathbf{x},t)$ of an infinite incompressible fluid of kinematic viscosity ν may be written, after elimination of the pressure term,[3] in the tensor form

$$\left(\frac{\partial}{\partial t}-\nu\nabla^2\right)u_i(\mathbf{x},t)=-\tfrac{1}{2}P_{imn}(\boldsymbol{\nabla})[u_m(\mathbf{x},t)u_n(\mathbf{x},t)], \tag{11.28}$$

where

$$P_{imn}(\boldsymbol{\nabla})=\left(\delta_{i,m}-\nabla^{-2}\frac{\partial^2}{\partial x_i\partial x_m}\right)\frac{\partial}{\partial x_n} +\left(\delta_{i,n}-\nabla^{-2}\frac{\partial^2}{\partial x_i\partial x_n}\right)\frac{\partial}{\partial x_m},$$

and

$$\nabla^{-2}f(\mathbf{x})\equiv-(4\pi)^{-1}\int|\mathbf{x}-\mathbf{y}|^{-1}f(\mathbf{y})d^3y$$

for any f. We may treat the incompressible turbulence problem in direct analogy to the foregoing analysis by taking a collection of flow systems with individual velocity fields $u^{[n]}(\mathbf{x},t)$ and considering the model equation[35]

$$\left(\frac{\partial}{\partial t}-\nu\nabla^2\right)u_i{}^\alpha(\mathbf{x},t) =-\tfrac{1}{2}M^{-\frac{1}{2}}P_{inm}(\nabla)\sum_\beta\phi_{\alpha,\beta,\alpha-\beta}[u_n{}^\beta(\mathbf{x},t)u_m{}^{\alpha-\beta}(\mathbf{x},t)], \tag{11.29}$$

where the $u_i{}^\alpha(x,t)$ are the collective velocity fields.

The final equations for the random coupling model

[34] Only terms involving solely diagonal elements of the Green's function matrix are of leading order ($M\to\infty$). Thus, for example, the variation in $u_{-\alpha}$ induced by the perturbation terms in the equation of motion for u_β does not contribute in the limit.

[35] We use superscripts to label individual and collective quantities here, in order to avoid possible confusion with tensor indices.

which result from Eq. (11.29) are similar to those for Burgers' equation, but more complicated. In the case of homogeneous turbulence, they take their simplest form when transformed to correspond to a representation of the velocity field by spatial Fourier modes. They are then identical with equations for homogeneous turbulence derived previously by a different method.[36] The earlier derivation exploited the fact that the Fourier amplitudes of a homogeneous field have statistical properties which closely resemble those of the collective coordinates used in the present paper (cf. Sec. 3). Unlike the present approach, which involves no geometrical symmetry restrictions and which may be extended to fully bounded flows, the earlier treatment is valid only in the homogeneous case. A discussion of the energy dynamics of the random coupling model is given in Sec. 4 of the first reference cited in footnote 36.

We wish, finally, to give a very brief discussion of turbulent convection, which will serve to illustrate a point raised at the end of Sec. 9. Let $\psi(\mathbf{x},t)$ represent the zero-mean fluctuations in the concentration of marked particles carried along with an incompressible turbulent flow which obeys Eq. (11.28). Then $\psi(\mathbf{x},t)$ satisfies

$$\left(\frac{\partial}{\partial t}-\kappa\nabla^2\right)\psi(\mathbf{x},t)=-u_i(\mathbf{x},t)\frac{\partial\psi(\mathbf{x},t)}{\partial x_i}, \quad (11.30)$$

where κ is the molecular diffusivity. If $\psi_{[n]}(\mathbf{x},t)$ and $\psi_\alpha(\mathbf{x},t)$ represent, respectively, the individual and collective fields for a collection of flows, the model equation corresponding to Eq. (11.30) is

$$\left(\frac{\partial}{\partial t}-\kappa\nabla^2\right)\psi_\alpha(\mathbf{x},t)=-M^{-\frac{1}{2}}\sum_\beta \phi_{\alpha,\beta,\alpha-\beta} \times u_i^\beta(\mathbf{x},t)\frac{\partial\psi_{\alpha-\beta}(\mathbf{x},t)}{\partial x_i}, \quad (11.31)$$

where Eqs. (11.5) and (11.6) are satisfied.

The random coupling model equations which result from Eq. (11.31), under Gaussian initial conditions of the form we have taken before, are

$$\left(\frac{\partial}{\partial t}-\kappa\nabla_x^2+\bar{u}_i(\mathbf{x},t)\frac{\partial}{\partial x_i}\right)G(\mathbf{x},t\,|\,\mathbf{x}',t')$$

$$=\int_{t'}^{t}ds\int d^3y U_{ij}(\mathbf{x},t;\mathbf{y},s)\frac{\partial G(\mathbf{x},t\,|\,\mathbf{y},s)}{\partial x_i}\frac{\partial G(\mathbf{y},s\,|\,\mathbf{x}',t')}{\partial y_j},$$

$$G(\mathbf{x},t'\,|\,\mathbf{x}',t')=\delta(\mathbf{x}-\mathbf{x}'), \quad (11.32)$$

and

$$\left(\frac{\partial}{\partial t}-\kappa\nabla_x^2+\bar{u}_i(\mathbf{x},t)\frac{\partial}{\partial x_i}\right)\Psi(\mathbf{x},t;\mathbf{x}',t')$$

$$=\frac{\partial}{\partial x_i}\int_{t_0}^{t'}ds\int d^3y U_{ij}(\mathbf{x},t;\mathbf{y},s)G(\mathbf{x}',t'\,|\,\mathbf{y},s) \times\frac{\partial\Psi(\mathbf{x},t;\mathbf{y},s)}{\partial y_j}+\frac{\partial}{\partial x_i}\int_{t_0}^{t}ds\int d^3y U_{ij}(\mathbf{x},t;\mathbf{y},s) \times G(\mathbf{x},t\,|\,\mathbf{y},s)\frac{\partial\Psi(\mathbf{x}',t';\mathbf{y},s)}{\partial y_j}, \quad (11.33)$$

where

$$\bar{u}_i(\mathbf{x},t)=\langle u_i^{[n]}(\mathbf{x},t)\rangle,$$

$$U_{ij}(\mathbf{x},t;\mathbf{x}',t')=\langle u_i^{[n]\prime}(\mathbf{x},t)u_j^{[n]\prime}(\mathbf{x}',t')\rangle,$$

$$\Psi(\mathbf{x},t;\mathbf{x}',t')=\langle\psi_{[n]}(\mathbf{x},t)\psi_{[n]}(\mathbf{x}',t')\rangle,$$

and $G(\mathbf{x},t\,|\,\mathbf{x}',t')$ is the mean diagonal Green's function for the concentration field.[37] We have assumed $\langle\psi_{[n]}(\mathbf{x},t)\rangle=0$, a condition which is preserved by the equations of motion. A detailed study of the consequences of these equations when the velocity field is statistically homogeneous has been made by Roberts,[38] who derives the equations for this case by methods related to those of the references cited in footnote 36. Another case has been discussed by the present author.[39]

In accord with the discussion in Sec. 9, the random coupling equations for turbulent convection involve only $\bar{u}_i(\mathbf{x},t)$ and the covariance tensor $U_{ij}(\mathbf{x},t;\mathbf{x}',t')$, regardless of the distribution of the fluctuating part of the velocity field. Suppose, now, we ask how the higher statistical structure of the velocity field can be incorporated in higher stochastic models for the convection problem. If this structure were known explicitly, we could, in principle, insert the associated cumulants in the non-Gaussian terms, of the type in Eq. (9.4), which contribute in the higher models. An alternative procedure is to assume Gaussian initial conditions for both the concentration field and the fluctuating velocity field and then treat Eqs. (11.29) and (11.31) as a simultaneous set, making the ϕ's identical in the two equations. The sequence of higher models for this problem would commence with that of Sec. 7, and the non-Gaussian diagrams would never arise. The assumption of Gaussian initial conditions often may be physically plausible, particularly if the flow has persisted long

[36] R. H. Kraichnan, J. Fluid Mech. 5, 497 (1959); see also, *Second Symposium on Naval Hydrodynamics*, edited by R. Cooper (United States Government Printing Office, Washington, 1960). The equations corresponding to the random coupling model are called the "direct-interaction approximation" equations in these papers.

[37] $G(\mathbf{x},t\,|\,\mathbf{x}',t')d^3x$ is the probability that a marked particle introduced at $\mathbf{x}'$, t' is in d^3x at $\mathbf{x},t$.

[38] P. H. Roberts (to be published). [Issued also as Rept. HSN-2, Division of Electromagnetic Research, Institute of Mathematical Sciences, New York University (1960).]

[39] R. H. Kraichnan, in *Hydrodynamic Instability*, Vol. 13, *Proceedings of Symposia in Applied Mathematics*, edited by G. Birkhoff (American Mathematical Society, Providence, Rhode Island, to be published).

enough that the higher statistical structure of the velocity field is determined principally by the dynamics rather than by the cumulants of the initial distribution.

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APPENDIX A

The second relation in Eq. (3.12) may be written

$$\langle G_{\alpha,\alpha}(t)G_{\alpha,\alpha}{}^*(t)\rangle - \langle G_{\alpha,\alpha}(t)\rangle\langle G_{\alpha,\alpha}{}^*(t)\rangle = O(M^{-1}), \quad \text{(A.1)}$$

where we use $\langle G_{\alpha,\alpha}(t)\rangle = G(t)$. Let the left-hand side of Eq. (A.1) be expanded by iteration of Eq. (4.6). In each term of the expansion of $G_{\alpha,\alpha}(t)$ or $G_{\alpha,\alpha}{}^*(t)$, the sum of indices of the b factors is zero [cf. argument leading to Eq. (4.7)]. Consequently, $\langle G_{\alpha,\alpha}(t)\rangle\langle G_{\alpha,\alpha}{}^*(t)\rangle$ consists of terms of the form

$$(-i)^{r-s}M^{-(r+s)/2}\sum_{\beta,\cdots,\mu,\gamma,\cdots,\sigma}(\text{product of }\phi\text{'s}) \times\langle b_\beta\cdots b_\mu b_{-\beta-\cdots-\mu}\rangle\langle b_\gamma\cdots b_\sigma b_{-\gamma-\cdots-\sigma}\rangle t^{r+s}/r!s!, \quad \text{(A.2)}$$

where there are r factors b in the first average and s in the second. For each such term there will be a corresponding term

$$(-i)^{r-s}M^{-(r+s)/2}\sum_{\beta,\cdots,\mu,\gamma,\cdots,\sigma}(\text{product of }\phi\text{'s}) \times\langle b_\beta\cdots b_\mu b_{-\beta-\cdots-\mu}b_\gamma\cdots b_\sigma b_{-\gamma-\cdots-\sigma}\rangle t^{r+s}/r!s! \quad \text{(A.3)}$$

in the expansion of $\langle G_{\alpha,\alpha}(t)G_{\alpha,\alpha}{}^*(t)\rangle$, where the product of ϕ's is identical for given indices $\beta, \cdots, \gamma, \cdots$. Let the ϕ's be bounded. Then the difference of Eqs. (A.2) and (A.3) is bounded in magnitude by

$$M^{-(r+s)/2}|\,(\text{product of }\phi\text{'s})\,|_{\max}\sum_{\beta,\cdots,\mu,\gamma,\cdots,\sigma} \times|\langle b_\beta\cdots b_\mu b_{-\beta-\cdots-\mu}\rangle\langle b_\gamma\cdots b_\sigma b_{-\gamma-\cdots-\sigma}\rangle - \langle b_\beta\cdots b_\mu b_{-\beta-\cdots-\mu}b_\gamma\cdots b_\sigma b_{-\gamma-\cdots-\sigma}\rangle|\,t^{r+s}/r!s!. \quad \text{(A.4)}$$

It now follows straightforwardly from Eq. (9.3) (we take the general non-Gaussian case) that Eq. (A.4) is $O(M^{-1})$ if $|\,(\text{product of }\phi\text{'s})\,|_{\max}$ is independent of M ($M \to \infty$). Similar analysis establishes Eqs. (8.14) and (11.15), if the iteration solutions of Eqs. (8.9) and (11.12), respectively, are used to express the equations in terms of the parameters and initial values, whose statistical properties are prescribed. In these solutions it is convenient to let the mean amplitudes remain in the expansions as parameters.

The significance of Eq. (3.12) was discussed in the text. Equations (8.14) and (11.15) also may be understood qualitatively as consequences of the fact that the dynamical behavior of a collective degree of freedom is determined ($M \to \infty$) by interaction with an infinite number of other degrees of freedom: The dynamical coupling with any given few of the other degrees of freedom is infinitesimal in the limit, and this implies a corresponding weakness of statistical dependence.

On a Moving Boundary Problem

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An exact analytic solution is obtained for a uniformly expanding, neutral, infinitely conducting plasma sphere in an external uniform and constant magnetic field.

I. INTRODUCTION

THE standard techniques for the solution of boundary value problems arising in mathematical physics are well known. The introduction of a moving boundary into the physics usually precludes the achievement of an exact analytic solution of the problem and recourse to approximation methods is required.[1] In the case of a moving plane boundary a time-dependent translation of the embedding space immobilizes the boundary at the expense of the increased complexity of the differential equation. It is the aim of this work to present an example of a soluble moving boundary value problem in spherical coordinate geometry.

Consider a spherical region of space containing a neutral infinitely conducting plasma which has expanded to its present state from a point source. The external environment is free of current and charge densities but contains a magnetic field which at infinity is uniform and constant, $\mathbf{B}=B_0\hat{k}$. As the spherical region expands it both perturbs the external magnetic field and generates an external electric field. Within the spherical region there is neither an electric field nor a magnetic field. We wish to obtain an analytic representation of the configuration of the external electromagnetic field.

External to the spherical domain the electromagnetic fields satisfy the source free Maxwell equations (except for the source at infinity which produces the magnetic field B_0). We shall use the rationalized mks system of units. Since the external region is devoid of free charge density, a suitable gauge allows the electric and magnetic fields to be derived from the vector potential $\mathbf{A}$, i.e., $\mathbf{E}=-\partial\mathbf{A}/\partial t$ and $\mathbf{B}=\nabla\times\mathbf{A}$. The vector potential of the original field written in spherical coordinates is $\mathbf{A}_0=\frac{1}{2}B_0 r\sin\theta\hat{\phi}$. Thus, it is sufficient to choose the vector potential $\mathbf{A}$ in the form $\mathbf{A}=W(r,t)\sin\theta\phi$. The differential equation for W obtained from the set of Maxwell's equations is

$$r^{-1}\partial^2(rW)/\partial r^2-2r^{-2}W-c^{-2}\partial^2W/\partial t^2=0. \tag{1}$$

This equation is to be solved in the external region $r>R(t)$ subject to boundary and initial conditions.

[1] Philip M. Morse and Herman Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, Chap. 9.

The initial conditions are

$$t=0: \qquad W=\tfrac{1}{2}B_0 r, \tag{2}$$

$$\partial W/\partial t=0. \tag{3}$$

The first initial condition states that the initial value of W is that of a uniform and constant magnetic field. The second initial condition states that there is no initial electric field. Boundary conditions must be imposed at the spherical surface $r=R(t)$ and at infinity. Because of the finite propagation velocity the magnetic field at infinity will remain undisturbed for all finite times. Further, no incoming wave-type solutions are permitted. Thus, for all finite times

$$r\to\infty, \quad W\to\tfrac{1}{2}B_0 r. \tag{4}$$

The boundary conditions at the expanding spherical surface must include the effects of the boundary motion. These conditions are

$$r=R(t), \quad \delta B_r=0, \tag{5}$$

$$\delta E_r=\omega/\epsilon, \tag{6}$$

$$\delta(E_\varphi+\dot{R}B_\theta)=0, \tag{7}$$

$$\delta(B_\theta+c^{-2}\dot{R}E_\varphi)=\mu K_\varphi, \tag{8}$$

where $\dot{R}$ is the velocity of the expanding surface, δ signifies the jump across the surface, ω is the surface charge density, and K_φ is the φ component of the surface current density. On introducing the function W and recalling that there are no internal electromagnetic fields, we obtain the boundary conditions in the form

$$r=R(t): \qquad W=0, \tag{9}$$

$$\partial W/\partial t+\dot{R}r^{-1}\partial(rW)/\partial r=0. \tag{10}$$

Further, the conditions upon the surface densities are

$$\omega=0, \tag{11}$$

showing the absence of free charge on the expanding surface and

$$r=R(t): \qquad r^{-1}\partial(rW)/\partial r+c^{-2}\dot{R}\partial W/\partial t=-\mu K_\varphi/\sin\theta, \tag{12}$$

relating the surface current density to the function W.

II. SOLUTION

The problem of solving Eq. (1) subject to the initial conditions in Eqs. (2) and (3) and the boundary conditions in Eqs. (9) and (10) will be accomplished by transform theory. We introduce a new dependent variable $V=r^{\frac{1}{2}}W$, whence Eq. (1) assumes the form

$$\partial^2V/\partial r^2+r^{-1}\partial V/\partial r-(3/2r)^2V-c^{-2}\partial^2V/\partial t^2=0. \quad (13)$$

The complex Laplace transform $\Phi(r,p)$ of the function $V(r,t)$ is introduced by

$$\Phi(r,p)=(2\pi)^{-\frac{1}{2}}\int_0^\infty V(r,t)e^{ipt}dt, \quad p=u+iv. \quad (14)$$

This transform is valid in the half-plane $v>v_0$, since V is of the exponential type, $V=O(e^{v_0|t|})$ and possesses an inverse

$$V(r,t)=(2\pi)^{-\frac{1}{2}}\int_{ia-\infty}^{ia+\infty}\Phi(r,p)e^{-ipt}dp, \quad a>v_0. \quad (15)$$

The differential equation satisfied by Φ is found from Eq. (13) and the initial conditions in Eqs. (2) and(3):

$$\partial^2\Phi/\partial r^2+r^{-1}\partial\Phi/\partial r+[(p/c)^2-(3/2r)^2]\Phi=\tfrac{1}{2}ip(2\pi)^{-\frac{1}{2}}c^{-2}B_0r^{\frac{3}{2}}. \quad (16)$$

Its solution may be written at once:

$$\Phi(r,p)=p^{-\frac{1}{2}}M(p)H_{\frac{3}{2}}^{(1)}(rp/c)+p^{-\frac{1}{2}}N(p)H_{\frac{3}{2}}^{(2)}(rp/c)+\tfrac{1}{2}i(2\pi)^{-\frac{1}{2}}p^{-1}B_0r^{\frac{3}{2}}, \quad (17)$$

where M and N are arbitrary functions of p determined from the boundary conditions in Eqs. (9) and (10), and $H_{\frac{3}{2}}$ is the Hankel function of order $\frac{3}{2}$. Since $H_{\frac{3}{2}}^{(2)}$ gives rise to incoming waves, we set $N=0$. The solution to Eq. (1) now may be written in the form

$$W(r,t)=\tfrac{1}{2}B_0r+r^{-1}\int_{ia-\infty}^{ia+\infty}dpM(p)p^{-1}(1+ic/rp)\times\exp[-ip(t-r/c)], \quad r>R(t). \quad (18)$$

This is actually the solution for a fixed domain where $M(p)$ is the transform of a boundary condition applied at $r=0$.

The moving boundary condition in Eq. (9) requires the satisfaction of

$$\tfrac{1}{2}B_0R^2+\int dpM(p)p^{-1}(1+ic/Rp)\times\exp[-ip(t-R/c)]=0. \quad (19)$$

Thus, the moving boundary condition is satisfied by matching it with an equivalent boundary condition at $r=0$. Since the sphere moves with a radial velocity w less than the velocity of light c, we have

$$R=\int_0^t wdt<\int_0^t cdt=ct,$$

or $t-R/c>0$. Thus, the contour in the integral of Eq. (19) may be closed by an infinite semicircle in the lower half plane and the integral evaluated by the method of residues.

Explicit evaluation of this rather awkward integral equation, Eq. (19), may be accomplished in the special case of a uniform expansion. Choosing the simple model of constant radial velocity $R=wt$ yields

$$M=-3B_0w^2(2\pi i)^{-1}(2+c/w)^{-1}(1-w/c)^{-2}p^{-2}, \quad (20)$$

whence the complete solution of Eq. (1) may be obtained by inserting Eq. (20) into Eq. (18) and evaluating the integral. On recalling that the interior region is devoid of electromagnetic fields, the solution may finally be written in the form

$$W(r,t)=\begin{cases}0, & r<wt\\ \tfrac{1}{2}B_0r-B_0\dfrac{w^3t^3}{2r^2}\left(\dfrac{1-r/ct}{1-w/c}\right)^2\left(\dfrac{1+2r/ct}{1+2w/c}\right), & wt<r<ct,\\ \tfrac{1}{2}B_0r, & ct<r.\end{cases} \quad (21)$$

It may also be noted that this special case of the uniform expansion falls within the conical flow techniques. From symmetry considerations one seeks a solution of the form $W=r^nF(r/ct)$. Substitution into the differential equation, Eq. (1), yields an explicitly solvable ordinary differential equation whose solution, upon application of the boundary conditions, is given by Eq. (21).

III. CONCLUSION

A complete solution of the uniform radial expansion of a neutral, infinitely conducting plasma sphere has been obtained. The electromagnetic fields are derived by forming the appropriate derivatives of W while the surface current density is obtained from Eq. (12). It may be seen immediately that the electromagnetic fields are perturbed only within the domain extending from the surface of the expanding plasma sphere $r=wt$ to the surface of the expanding information sphere $r=ct$. External to the sphere $r=ct$ only the initial constant and uniform magnetic field is to be found.

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