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Random Walks on Lattices. II

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Formulas are obtained for the mean first passage times (as well as their dispersion) in random walks from the origin to an arbitrary lattice point on a periodic space lattice with periodic boundary conditions. Generally this time is proportional to the number of lattice points.

The number of distinct points visited after n steps on a k-dimensional lattice (with $k \geq 3$) when n is large is $a_1 n + a_2 n^{\frac{1}{2}} + a_3 + a_4 n^{-\frac{1}{2}} + \cdots$. The constants $a_1 - a_4$ have been obtained for walks on a simple cubic lattice when $k = 3$ and a_1 and a_2 are given for simple and face-centered cubic lattices. Formulas have also been obtained for the number of points visited r times in n steps as well as the average number of times a given point has been visited.

The probability $F(c)$ that a walker on a one-dimensional lattice returns to his starting point before being trapped on a lattice of trap concentration c is $F(c) = 1 + [c/(1 - c)] \log c$.

Most of the results in this paper have been derived by the method of Green's functions.

A NUMBER of problems in solid-state physics are directly or indirectly related to various aspects of random walks on periodic space lattices. The theory of such random walks on infinite lattices was first discussed by Polya[1] who was especially concerned with the effect of dimensionality on the probability that a walker starting at a given point eventually returns to that point. Some other types of problems which are of special interest involve the average time required by a walker to go from a given lattice point to another preassigned point for the first time and with the average number of distinct points occupied in a walk of a given number of steps. Results on these topics as well as the effect of a small number of lattice defects on random walks have been discussed in the first paper of this series.[2]

That paper is concerned mainly with random walks which involve jumps to nearest-neighbor lattice points only. Many of the results are generalized here to be applicable to walks which involve steps to more distant neighbors. We also discuss the average number of points occupied k times in an n-step walk as well as the number of times a given point has been occupied in such a walk. The average number of points occupied in an n-step walk was first estimated by Dvoretsky and Erdös,[3] further analysis having been made by Vineyard[4] and one of the authors.[2] Repeated occupancy was first considered by Erdös and Taylor.[5]

Green's function techniques and Tauberian theorems are the main mathematical tools used in this paper. Although emphasis is placed on walks in which steps are taken at regular time intervals, the generalization to those in which the steps are taken at random times is developed in Sec. V.

We also discuss the effect of traps of a given con-

[1] G. Polya, Math. Ann. **84**, 149 (1921).
[2] E. W. Montroll, Proc. Symp. Appl. Math. Am. Math. Soc. **16**, 193 (1964).
[3] A. Dvoretzky and E. Erdos, Proc. 2nd Berkeley Sympos. Math. Stat. and Prob., (University of California Press, Berkeley, 1951), p. 33.
[4] G. H. Vineyard, J. Math. Phys. **4**, 1191 (1963).
[5] P. Erdos and S. J. Taylor, Acta Math. Acad. Sci. Hung. **11**, 137 (1960).

centration on the probability of a walker on a one-dimensional lattice returning to his starting point before being trapped.

Since the first draft of this article was completed, a book by Spitzer[6] has appeared which contains a discussion of some of the topics included here.

I. LATTICE GREEN'S FUNCTIONS AND RANDOM-WALK GENERATING FUNCTIONS

We begin by studying discrete random walks on lattices with periodic boundary conditions (i.e., toroidal lattices), and in particular will assume that there exists an integer N such that the lattice points $\mathbf{s} = (s_1, s_2, \cdots, s_k)$ satisfy

$$(s_1 + j_1N, s_2 + j_2N, \cdots, s_k + j_kN) = (s_1, s_2, \cdots, s_k)$$

when the j's are integers.

There are N^k distinct lattice points on our k-dimensional lattice. Let $P_n(\mathbf{s})$ be the probability that the random walker is at a point $\mathbf{s}$ after the nth step. In view of the periodic boundary conditions,

$$P_n(s_1 + j_1N, s_2 + j_2N, \cdots, s_k + j_kN) = P_n(\mathbf{s}), \quad \text{(I.1)}$$

when the j's are integers. The $\{P_n(\mathbf{s})\}$ satisfy the recursion formula

$$P_{n+1}(\mathbf{s}) = \sum_{\mathbf{s}'} p(\mathbf{s} - \mathbf{s}')P_n(\mathbf{s}'), \quad \text{(I.2)}$$

if $p(\mathbf{s})$ represents the probability that any step results in a vector displacement $\mathbf{s}$ by a walker. We find the Fourier expansion of $p(\mathbf{s})$

$$\lambda(2\pi\mathbf{r}/N) = \sum_{\mathbf{s}} p(\mathbf{s}) \exp(2\pi i\mathbf{r}\cdot\mathbf{s}/N), \quad \text{(I.3)}$$

which we call the structure function of the walk, to be of considerable importance. In particular

$$\sum_{\mathbf{s}} p(\mathbf{s}) = 1 \quad \text{and} \quad \lambda(0) = 1 \quad \text{(I.4)}$$

when walkers are conserved; i.e., when walkers are neither created nor destroyed in the walk. The reader can easily verify that

$$\lambda(\boldsymbol{\vartheta}) = \begin{cases} (c_1 + c_2 + \cdots + c_k)/k \\ \quad \text{for } k\text{-D simple cubic lattice} \\ (c_1c_2 + c_2c_3 + c_3c_1)/3 \\ \quad \text{for 3-D face-centered cubic lattice} \\ c_1c_2c_3, \\ \quad \text{for 3-D body-centered cubic lattice,} \end{cases} \quad \text{(I.5)}$$

where

$$c_j = \cos\vartheta_j \quad \text{and} \quad \vartheta_j = 2\pi r_j/N. \quad \text{(I.5a)}$$

Properties of random walks can be described effectively through the random-walk generating function

$$P(\mathbf{s}, z) = \sum_0^\infty z^n P_n(\mathbf{s}). \quad \text{(I.6)}$$

We restrict ourselves now to the initial condition

$$P_0(\mathbf{s}) = \delta_{\mathbf{s},0} \quad \text{(I.7)}$$

which corresponds to walks which start from the origin, $\mathbf{s} = 0$. By multiplying (2) by z^n, summing over all n, and applying (7), one finds that $P(\mathbf{s}, z)$ satisfies the Green's function equation

$$P(\mathbf{s}, z) - z\sum_{\mathbf{s}'} p(\mathbf{s} - \mathbf{s}')P(\mathbf{s}', z) = \delta_{\mathbf{s},0}. \quad \text{(I.8)}$$

This equation can be solved for our generating function $P(\mathbf{s}, z)$ by considering the function

$$u(z, 2\pi\mathbf{r}/N) = \sum_{\mathbf{s}} P(\mathbf{s}, z) \exp(2\pi i\mathbf{r}\cdot\mathbf{s}/N). \quad \text{(I.9)}$$

If we multiply (8) by $\exp(2\pi i\mathbf{s}\cdot\mathbf{r}/N)$, sum over $\mathbf{s}$ and employ (9) and (3) we find

$$u(z, 2\pi\mathbf{r}/N) = \{1 - z\lambda(2\pi\mathbf{r}/N)\}^{-1}. \quad \text{(I.10)}$$

Since $P(\mathbf{s}, z)$ is the Fourier inverse of $u(z, 2\pi\mathbf{r}/N)$, we find

$$P(\mathbf{s}, z) = N^{-k}\sum_{\mathbf{r}} \frac{\exp(-2\pi i\mathbf{r}\cdot\mathbf{s}/N)}{1 - z\lambda(2\pi\mathbf{r}/N)}. \quad \text{(I.11)}$$

In the case of an infinite lattice, $N \to \infty$ and

$$P(\mathbf{s}, z) = \frac{1}{(2\pi)^k}\int_{-\pi}^{\pi}\cdots\int \frac{\exp(-i\mathbf{s}\cdot\boldsymbol{\vartheta})\, d^k\boldsymbol{\vartheta}}{1 - z\lambda(\boldsymbol{\vartheta})}. \quad \text{(I.12)}$$

From this it is clear that

$$P_n(\mathbf{s}) = \frac{1}{(2\pi)^s}\int_{-\pi}^{\pi}\cdots\int [\lambda(\boldsymbol{\vartheta})]^n e^{-i\mathbf{s}\cdot\boldsymbol{\vartheta}}\, d^k\boldsymbol{\vartheta}. \quad \text{(I.13)}$$

Also since we assume walkers to be conserved

$$\sum_{\mathbf{s}} P_n(\mathbf{s}) = 1, \quad \text{(I.14a)}$$

and

$$\sum_{\mathbf{s}} P(\mathbf{s}, z) = (1 - z)^{-1}. \quad \text{(I.14b)}$$

In all the analysis above we assume $|z| \leq 1$.

We will find it expedient to separate out the singular and nonsingular parts of $P(\mathbf{s}, z)$ by writing

$$P(\mathbf{s}, z) = (1 - z)N^{-k} + \varphi(\mathbf{s}, z), \quad \text{(I.15)}$$

where

$$\varphi(\mathbf{s}, z) = N^{-k}\sum_{\mathbf{r}}{}' \frac{\exp(2\pi i\mathbf{r}\cdot\mathbf{s}/N)}{1 - z\lambda(2\pi\mathbf{r}/N)}, \quad \text{(I.16)}$$

[6] F. Spitzer, *Principles of Random Walks* (D. Van Nostrand, Inc., Princeton, New Jersey, 1964).

in which the prime indicates that the term with $r_1 = r_2 = \cdots = r_k = 0$ is to be omitted. In general, when the limit $N \to \infty$ is taken, the sum can be replaced by an integral. Although the resulting integral may be a singular function of z the singularity is weaker than $(1 - z)^{-1}$ as we show later.

We will also be interested in the properties of the first passage time, and for this purpose we define $F_n(\mathbf{s})$ to be the probability that a random walker reaches the point $\mathbf{s}$ for the *first time* at step n. The generating function of the $F_n(\mathbf{s})$ will be denoted by $F(\mathbf{s}, z)$:

$$F(\mathbf{s}, z) = \sum_{n=1}^{\infty} F_n(\mathbf{s}) z^n. \tag{I.17}$$

It is possible to relate the $F_n(\mathbf{s})$ to the $P_n(\mathbf{s})$ since, if the random walker is at step n he must first have reached there at some step j and then returned to s in $n - j$ steps. Taking account of the initial condition of Eq. (I.3), we find

$$P_n(\mathbf{s}) = \delta_{n,0}\delta_{s,0} + \sum_{j=1}^{n} F_j(\mathbf{s}) P_{n-j}(0)$$

The generating functions therefore satisfy

$$F(\mathbf{s}, z) = [P(\mathbf{s}, z) - \delta_{s,0}]/P(0, z). \tag{I.18}$$

The probability that the walker reaches point s at some time is just $F(s, 1)$. For $N < \infty$ the probability of reaching any point on the lattice is one, independent of the dimension. When $N = \infty$ the probability of a return to the origin is $1 - [F(0, 1)]^{-1}$ In one and two dimensions $F(0, 1) = \infty$ and the walker returns to the origin with probability one. In higher dimensions the return to the origin occurs with probability less than one. The same results are true for the first passage to any point $\mathbf{s}$.

Another function that will be useful later is $F_n^{(r)}(\mathbf{s})$, the probability that the random walker reaches $\mathbf{s}$ for the rth time at step n. This function satisfies the recurrence formula

$$F_n^{(r)}(\mathbf{s}) = \sum_{j=1}^{n} F_{n-j}^{(r-1)}(\mathbf{s}) F_j(0), \tag{I.19}$$

and its generating function $F^{(r)}(\mathbf{s}, z)$ is therefore given by

$$F^{(r)}(\mathbf{s}, z) = [F(0, z)]^{r-1} F(\mathbf{s}, z) = \sum_{n=1}^{\infty} F_n^{(r)}(\mathbf{s}) z^n. \tag{I.20}$$

II. STATISTICS OF FIRST-PASSAGE TIME

The first results to be given will be those related to first-passage times. Let $\langle n^j(\mathbf{s})\rangle$ be the jth moment of the first-passage time to reach point $\mathbf{s}$. In terms of $F(\mathbf{s}, z)$, $\langle n^j(\mathbf{s})\rangle$ can be written

$$\langle n^j(\mathbf{s})\rangle = (z\, \partial/\partial z)^j F(\mathbf{s}, z)]_{z=1}. \tag{II.1}$$

In particular, if we substitute the representation of Eq. (II.15) for $P(\mathbf{s}, z)$ into (II.18) we find, for the first two moments

$$\langle n(\mathbf{s})\rangle = \begin{cases} N^k[\varphi(0, 1) - \varphi(\mathbf{s}, 1)], & \mathbf{s} \neq 0, \quad \text{(II.2a)} \\ N^k, & \mathbf{s} = 0, \quad \text{(II.2b)} \end{cases}$$

$$\langle n^2(\mathbf{s})\rangle = [2N^k\varphi(0, 1) + 1]\langle n(\mathbf{s})\rangle + 2N^k\left[\frac{\partial\varphi(0, z)}{\partial z} - \frac{\partial\varphi(\mathbf{s}, z)}{\partial z}\right]_{z=1} \quad \text{if } \mathbf{s} \neq 0, \tag{II.3a}$$

$$\langle n^2(0)\rangle = 2N^{2k}\varphi(0, 1) + N^k. \tag{II.3b}$$

Notice that *the expected number of steps required to return to the origin is* N^k, the total number of lattice points, independently of the structure of the lattice. The second moment of the expected number of steps required to return to the origin for the first time does depend on lattice structure as is indicated by the function $\varphi(0, 1)$. Moments of the number of steps to reach other points on the lattice for the first time all depend on the structure.

So far we have given formal results valid for any k-dimensional periodic lattice. In the next few paragraphs we shall illustrate the general theory by evaluating some of the relevant functions for particular lattices. In our evaluation we will need some analytic properties of the functions $\lambda(\boldsymbol{\vartheta})$ and $\varphi(\mathbf{r}, z)$ which appear in many of the formulas derived above. We shall be interested only in symmetric random walks, hence the expansion of $\lambda(\boldsymbol{\vartheta})$ in a neighborhood of the origin is

$$\lambda(\boldsymbol{\vartheta}) = 1 - \frac{1}{2}\sum_{1}^{k} \sigma_i^2\vartheta_i^2 + O(\vartheta^4), \tag{II.4}$$

where

$$\sigma_i^2 = \sum_m m_i^2 p(m). \tag{II.5}$$

We will make use of $\varphi(\mathbf{s}, z)$ for an infinite lattice in the limit $z = 1^-$. The expression for $\varphi(\mathbf{s}, z)$ when $N = \infty$ is

$$\varphi(\mathbf{s}, z) = \frac{1}{(2\pi)^k} \times \int_{-\pi}^{\pi} \cdots \int \frac{\exp(i\boldsymbol{\vartheta}\cdot\mathbf{s})\, d^k\boldsymbol{\vartheta}}{1 - z\lambda(\boldsymbol{\vartheta})} = P(\mathbf{s}, z). \tag{II.6}$$

The function $\varphi(\mathbf{s}, 1)$ is singular in one and two dimensions. We can see this by considering the contribution to $\varphi(\mathbf{s}, 1)$ from a neighborhood of the origin $\boldsymbol{\vartheta} = 0$,

$$\int \cdots \int \frac{d^k\boldsymbol{\vartheta}}{\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2}. \tag{II.7}$$

If the integrand is transformed to polar coordinates, there arise contributions of the form

$$\int \cdots \int \frac{r^{k-1}}{r^2}\, dr, \tag{II.8}$$

which diverges in one and two dimensions, but remains finite in higher dimensions. We will be interested in the behavior of $\varphi(\mathbf{s}, z)$ for $\mathbf{s} = 0$ and $\mathbf{s} = (s_1^2 + \cdots + s_k^2)^{\frac{1}{2}}$ large but not large enough to violate the condition $\mathbf{s} \ll N^k$. It will be demonstrated that the properties of $\langle n(\mathbf{s})\rangle/N^k$ can be obtained fairly simply for large distances from the origin.

Let us begin by decomposing the integral defining $\varphi(s, z)$ into two parts:

$$\varphi(\mathbf{s}, z) = \frac{1}{(2\pi)^k} \int_{-\pi}^{\pi} \cdots \int \frac{\exp(i\boldsymbol{\vartheta}\cdot\mathbf{s})\, d^k\boldsymbol{\vartheta}}{1 - z + \frac{1}{2}z(\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2)}$$

$$+ \frac{1}{(2\pi)^k} \int_{-\pi}^{\pi} \cdots \int e^{i\boldsymbol{\vartheta}\cdot\mathbf{s}} \left\{ \frac{1}{1 - z\lambda(\vartheta)} - \frac{1}{1 - z + \frac{1}{2}z(\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2)} \right\} d^k\boldsymbol{\vartheta}$$

$$= \varphi_1(\mathbf{s}, z) + \varphi_2(\mathbf{s}, z). \tag{II.9}$$

The singularity in one and two dimensions at $z = 1$ comes from the function $\varphi_1(\mathbf{s}, z)$ since the integral for $\varphi_2(\mathbf{s}, 1)$ has the form

$$\int \cdots \int r^{k-1}\, dr$$

at the origin of θ space. In higher dimensions both $\varphi_1(\mathbf{s}, z)$ and $\varphi_2(\mathbf{s}, z)$ approach zero as $\mathbf{s} \to \infty$, but

$$\lim_{\mathbf{s}\to\infty} [\varphi_2(\mathbf{s}, 1)/\varphi_1(\mathbf{s}, 1)] = 0. \tag{II.10}$$

This limit can be established by examining the behavior of the integrands in the neighborhood of $\boldsymbol{\vartheta} = 0$, which gives the principal contribution in the range of large $\mathbf{s}$. A detailed justification is given in Appendix A. We therefore see that the significant analytic properties of $\varphi(\mathbf{s}, z)$ are contained in $\varphi_1(\mathbf{s}, z)$ for large $\mathbf{s}$.

We shall recast the form of this function as a Laplace transform and begin by using the identity

$$u^{-1} = \int_0^\infty e^{-ut}\, dt$$

to rewrite it as

$$\varphi_1(\mathbf{s}, z) = \int_0^\infty e^{-(1-z)t}\, dt \times \prod_{i=1}^{k} \left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(i\vartheta_i s_i - \tfrac{1}{2}zt\sigma_i^2\vartheta_i^2)\, d\vartheta_i \right\}, \tag{II.11}$$

where the interchange of orders of integration can be justified in detail. Thus $\varphi_1(\mathbf{s}, z)$ can be expressed as a Laplace transform

$$\varphi_1(\mathbf{s}, z) = \int_0^\infty e^{-(1-z)t} F(z, t)\, dt, \tag{II.12}$$

where $F(z, t)$ is the product of integrals in Eq. (II.11). Since each of the integral factors of $F(z, t)$ is analytic in z at $z = 1$, we may expand $F(z, t)$ in a Taylor series around $z = 1$,

$$F(z, t) = F(1, t) + (z - 1)[\partial F/\partial z]_{z=1} + \cdots. \tag{II.13}$$

Since we are interested in the behavior of $\varphi_1(\mathbf{s}, z)$ at $z = 1$ we can invoke an Abelian theorem for Laplace transforms[7] which states in the present context that the behavior of $\varphi(\mathbf{s}, z)$ at $z = 1$ is determined by the behavior of $F(z, t)$ at $t = \infty$.

To determine this behavior we note that as $t \to \infty$ the integrand of each of the integrals in $\varphi_1(\mathbf{s}, z)$ is peaked sharply at the origin with negligible contribution coming from values of ϑ_i greater than $2/\sigma_i t^{\frac{1}{2}} z^{\frac{1}{2}}$. Hence the ranges of integration on the ϑ integrals $(-\pi, \pi)$ can, as $t \to \infty$ be replaced by $(-\infty, \infty)$ so that

$$F(z, t) \sim \prod_{i=1}^{k} (2\sigma_i^2\pi t z)^{-\frac{1}{2}} \exp(-s_i^2/2zt\sigma_i^2)$$

and

$$F(1, t) \sim [\sigma_1 \cdots \sigma_k (2\pi t)^{k/2}]^{-1} \exp(-\lambda^2/2t), \tag{II.14a}$$

where

$$\lambda^2 = \sum_{i=1}^{k} (s_i/\sigma_i)^2. \tag{II.14b}$$

In one dimension we find

$$\varphi_1(s, z) \sim \frac{1}{\sigma(2\pi)^{\frac{1}{2}}} \int_0^\infty e^{-(1-z)t - (s^2/2t\sigma^2)} t^{-\frac{1}{2}}\, dt$$

$$= \frac{2^{\frac{1}{2}} s^{\frac{1}{2}}}{\pi^{\frac{1}{2}}\sigma^{\frac{1}{2}}(1 - z)^{\frac{1}{4}}} K_{\frac{1}{2}}\left(\frac{s}{\sigma}[2(1 - z)]^{\frac{1}{2}}\right)$$

$$= \frac{\exp\{-(s/\sigma)[2(1 - z)]^{\frac{1}{2}}\}}{\sigma[2(1 - z)]^{\frac{1}{2}}}, \tag{II.15}$$

where $K_{1/2}(x)$ is a Bessel function of the third kind of imaginary argument. The two-dimensional form $\varphi_1(\mathbf{s}, z)$ for $\lambda \neq 0$ is

$$\varphi_1(\mathbf{s}, z) \sim \frac{1}{2\pi\sigma_1\sigma_2} \int_0^\infty t^{-1} \exp\{-(1 - z)t - \lambda^2/2t\}\, dt$$

$$= \frac{1}{\pi\sigma_1\sigma_2} K_0(\lambda[2(1 - z)]^{\frac{1}{2}}). \tag{II.16}$$

[7] D. V. Widder, *The Laplace Transform* (Princeton University Press, Princeton, New Jersey, 1941).

When $\lambda = 0$ we may use an Abelian theorem for Laplace transforms[7] to show that it follows from the asymptotic form $F(1, t) \sim (2\pi\sigma_1\sigma_2 t)^{-1}$ that

$$\varphi_1(0, z) \sim -(1/2\pi\sigma_1\sigma_2) \log (1 - z) \qquad \text{(II.17)}$$

for $z \to 1^-$. In three dimensions and higher $\varphi_1(0, 1)$ is defined by a convergent integral and must be calculated numerically. For large λ^2 an asymptotic expression for $\varphi_1(\mathbf{s}, 1)$ is

$$\varphi_1(s, 1) \sim \frac{1}{(2\pi)^{k/2}\sigma_1 \cdots \sigma_k} \int_0^\infty e^{-\lambda^2/2t} t^{-k/2}\, dt$$

$$= \lambda^{2-k}\Gamma(\tfrac{1}{2}k - 1)/2\sigma_1 \cdots \sigma_k \pi^{k/2}. \qquad \text{(II.18a)}$$

The 3-D expression for $P(\mathbf{s}, z)$ as $z \to 1$ is

$$P(\mathbf{s}, z) \sim (2\pi\lambda\sigma_1\sigma_2\sigma_3)^{-1} \exp\{-\lambda[2(1 - z)]^{\frac{1}{2}}\}. \qquad \text{(II.18b)}$$

Let us now consider some results for specific lattices. The simplest case is that of a one-dimensional lattice with jumps to nearest neighbors with probability $\frac{1}{2}$. For this case we can calculate an explicit expression for[2] $P(s, z)$:

$$P(s, z) = \frac{1}{N} \sum_{r=0}^{N-1} \frac{\exp(2\pi irs/N)}{1 - z \cos(2\pi r/N)}$$

$$= \frac{(1 - z^2)^{-\frac{1}{2}}(U^s + U^{N-s})}{(1 - U^N)}, \qquad \text{(II.19a)}$$

where

$$U = z^{-1}\{1 - (1 - z^2)^{\frac{1}{2}}\}. \qquad \text{(II.19b)}$$

It is known that the mean recurrence time for return to the origin is infinite for an infinite lattice, even though the return probability[8] is 1. Likewise the expected time to reach any point is infinite although the probability of reaching any point is 1. This difficulty is avoided in the case of a finite lattice. Here, in contrast to the Polya case, return to the origin or to any lattice point occurs with probability one in any number of dimensions. We shall calculate the expected time to reach any point for the first time for nearest-neighbor jumps, and then present the generalization for different one-dimensional random walks, in the limit of large N. For the lattice with jumps to nearest neighbors only, we find[2] by an exact calculation starting from Eqs. (II.2a) and (II.19)

$$\langle n(s)\rangle = s(N - s). \qquad \text{(II.20)}$$

To treat the case of the general one-dimensional walk for which $N \gg \mathbf{s}$, we use Eqs. (II.2a) and (II.15) to find

$$\lim_{N\to\infty} \langle n(s)\rangle/N = \varphi(0, 1) - \varphi(s, 1)$$

$$\sim \lim_{s\to 1} [\varphi_1(0, z) - \varphi_1(s, z)] = s/\sigma^2. \qquad \text{(II.21)}$$

In the two-dimensional case, since

$$K_0\{\lambda[2(1 - z)]^{\frac{1}{2}}\} \sim -\tfrac{1}{2} \log (1 - z) - \log \lambda + O(1)$$

for large λ, we have the expression

$$\lim_{N\to\infty} \langle n(\mathbf{s})\rangle/N^2 \sim \frac{\log \lambda}{\pi\sigma_1\sigma_2}. \qquad \text{(II.22)}$$

For the symmetric random walk on a simple square lattice with jumps to nearest neighbors, $\sigma_1 = \sigma_2 = 2^{-\frac{1}{2}}$ and the mean passage time is

$$\lim_{N\to\infty} \frac{\langle n(\mathbf{s})\rangle}{N^2} = \frac{2 \log s}{\pi}. \qquad \text{(II.23)}$$

The three-dimensional first-passage time is given by

$$\lim_{N\to\infty} \frac{\langle n(\mathbf{s})\rangle}{N^3}$$

$$= \varphi(0, 1) - \frac{1}{2\pi\sigma_1\sigma_2\sigma_3\lambda} + \cdots, \quad \mathbf{s} \neq 0. \qquad \text{(II.24)}$$

It is interesting to note that, in one and two dimensions, the first term in the asymptotic expansion for the mean first-passage time depends only on λ and the σ_i and not on any further detailed description of the lattice. Furthermore, $\langle n(\mathbf{s})\rangle/N^k$ is an increasing function of λ for large λ in one and two dimensions. In three and higher dimensions the mean first-passage time depends in a detailed way on the lattice [through $\varphi(0, 1)$] and to a first approximation is a constant, independent of λ.

Calculation of the variances of the first passage times is considerably more difficult because, at the very least, the expression for the variance contains $\varphi(0, 1)$. For the one-dimensional random walk with jump probabilities of $\frac{1}{2}$ to either nearest neighbor, the detailed expansion of $P(s, z)$ around $z = 1$ is from Eq. (II.19)

$$P(s, z) = 1 - s(N - s)(1 - z) + \tfrac{1}{6}s(N - s)$$

$$\times (N^2 + sN - s^2 - 5)(1 - z)^2 + \cdots. \qquad \text{(II.25)}$$

From this expression we derive

$$\sigma^2(s) = \langle n^2(s)\rangle - \langle n(s)\rangle^2$$

$$= \tfrac{1}{3}s(N - s)[N^2 - 2s(N - s) - 2], \quad s \neq 0. \qquad \text{(II.26)}$$

For $s = 0$ we have

$$F(0, z) = 1 - [P(0, z)]^{-1} = 1 - N(1 - z)$$

$$+ \tfrac{1}{6}N(N^2 - 1)(1 - z)^2 - \cdots, \qquad \text{(II.27)}$$

[8] W. Feller, *An Introduction to Probability Theory and its Applications* (John Wiley & Sons, Inc., New York, 1951).

from which it follows that[2]

$$\sigma^2(0) = \tfrac{1}{3}N(N-1)(N-2). \qquad \text{(II.28)}$$

It is possible to derive an asymptotic value for $\sigma^2(0)$ for any 1-D transition probabilities by noticing that in the limit $N = \infty$, the principal contributions in

$$\varphi(0,1) = \frac{1}{N}\sum_{j=1}^{N-1}\left\{1-\lambda\left(\frac{2\pi j}{N}\right)\right\}^{-1}$$
$$= \frac{2}{N}\sum_{j=1}^{[\frac{1}{2}(N-1)]}\left\{1-\lambda\left(\frac{2\pi j}{N}\right)\right\}^{-1}$$
$$+\frac{1}{2N}[1+(-1)^N]\left\{1-\lambda\left(\frac{2\pi[\frac{1}{2}(N-1)]+2\pi}{N}\right)\right\}^{-1}$$

come from small j. We therefore expand $\lambda(2\pi j/N)$ according to Eq. (II.4) and find

$$\varphi(0,1) \sim \frac{N}{\pi^2\sigma_1^2}\sum_{j=1}^{[\frac{1}{2}(N-1)]} j^{-2}. \qquad \text{(II.29)}$$

In the limit of large N the series can be replaced by its sum to infinity $\frac{1}{6}\pi^2$, and the asymptotic expression for the variance becomes

$$\sigma^2(0) \sim N^3/3\sigma_1^2 \qquad \text{(II.30)}$$

in agreement with the special result given in Eq. (II.28). It is also possible to derive an expression for $\sigma^2(s)$ for $s \ll N$ by this technique. A calculation similar to the preceding serves to show that

$$\frac{\partial\varphi(0,1)}{\partial z} - \frac{\partial\varphi(s,1)}{\partial z} = \frac{Ns^2}{6\sigma_1^4}; \qquad \text{(II.31)}$$

hence the principal contribution to $\sigma^2(s)$ comes from the first term in the expression for $\langle n^2(s)\rangle$. Using the expression for $\varphi(0,1)$ given in Eq. (II.29) we find

$$\sigma^2(s) = (sN^3)/(3\sigma_1^4). \qquad \text{(II.32)}$$

It is shown in Appendix B that the asymptotic form for $\varphi(0,1)$ in the 2-D case as $N \to \infty$ is

$$\varphi(0,1) \sim (\pi\sigma_1\sigma_2)^{-1}\log N. \qquad \text{(II.33)}$$

Hence in 2D the variance in the return time to the origin is

$$\sigma^2(0) \sim (2/\pi\sigma_1\sigma_2)N^4\log N. \qquad \text{(II.34)}$$

The sum defining $\varphi(0,1)$ converges in three dimensions and greater. As $N \to \infty$, $\varphi(0,1)$ has the integral form (II.6). These integrals have been calculated by Watson[9] for cubic lattices. From the numerical values one obtains the following estimates of $\sigma^2(0)$ for the cubic lattices:

s.c. $\sigma^2(0)/N^6$

$$\sim \frac{2}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\vartheta}{1-\frac{1}{3}(c_1+c_2+c_3)} - 1 = 2.032,$$

f.c. $\sigma^2(0)/N^6$

$$\sim \frac{2}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\vartheta}{1-\frac{1}{3}(c_1c_2+c_2c_3+c_3c_1)} - 1 = 1.690,$$

b.c. $\sigma^2(0)/N^6$

$$\sim \frac{2}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\vartheta}{1-c_1c_2c_3} - 1 = 1.786.$$

It is of incidental interest that the expression for the variance

$$\sigma^2(0) = N^{2k}[2\varphi(0,1)-1] + N^k \qquad \text{(II.35)}$$

shows that, for $k \geq 3$,

$$\varphi(0,1) \geq \tfrac{1}{2}, \qquad \text{(II.36)}$$

a result which seems otherwise difficult to prove.

III. NUMBER OF POINTS VISITED r TIMES IN AN n-STEP WALK

We now turn to the statistics of the number of distinct lattice points visited during an n-step walk. We will be concerned mainly with the large n case, although some results will also be given for any integer n.

Let S_n be the average number of lattice points visited in an n-step walk. Then

$$S_n = 1 + \sum_{\mathbf{s}}{}' \{F_1(\mathbf{s}) + F_2(\mathbf{s}) + \cdots + F_n(\mathbf{s})\}, \qquad \text{(III.1)}$$

where the primed summation proceeds over all lattice points except the origin. The integer 1 represents the fact that the walker was originally at the origin. As before $F_j(\mathbf{s})$ is the probability that the walker arrives at $\mathbf{s}$ for the first time after the jth step. Hence the summand of (III.1) represents the probability that the point $\mathbf{s}$ has been occupied at least once in the first n steps.

It is convenient to define a quantity Δ_k by

$$\Delta_k = S_k - S_{k-1}, \qquad k = 1, 2, \cdots. \qquad \text{(III.2)}$$

Since $S_0 = 1$ and $S_1 = 2$ we find $\Delta_1 = 1$. Then

$$\Delta_n = \sum_{\mathbf{s}}{}' F_n(\mathbf{s}) = -F_n(0) + \sum_{\mathbf{s}} F_n(\mathbf{s}). \qquad \text{(III.3)}$$

[9] G. N. Watson, Quar. J. Math. Oxford, Ser. 10, 266 (1939).

Hence the generating function for Δ_k is

$$\Delta(z) = \sum_1^\infty z^n \Delta_n$$

$$= -\sum_1^\infty z^n F_n(0) + \sum_s \sum_{n=1}^\infty z^n F_n(\mathbf{s}), \quad \text{(III.4)}$$

so that

$$\Delta(z) = -F(0, z) + \sum_s F(\mathbf{s}, z). \quad \text{(III.5)}$$

However from Eq. (I.18)

$$F(\mathbf{s}, z) = \frac{P(\mathbf{s}, z) - \delta_{\mathbf{s},0}}{P(0, z)} \quad \text{(III.6)}$$

and

$$\Delta(z) = -1 + \sum_s \frac{P(\mathbf{s}, z)}{P(0, z)}. \quad \text{(III.7)}$$

Then Eq. (I.14b) implies

$$\Delta(z) = -1 + \{(1 - z)P(0, z)\}^{-1}. \quad \text{(III.8)}$$

The generating function $S(z)$ can be obtained immediately from this expression since

$$S_0 = 1,$$

$$S_1 = 1 + \Delta_1,$$

$$\cdots$$

$$S_n = 1 + \Delta_1 + \Delta_2 + \cdots + \Delta_n \quad \text{etc.}, \quad \text{(III.9)}$$

we find

$$S(z) = \frac{1}{1 - z} + \frac{z\Delta_1}{1 - z} + \frac{z^2\Delta_2}{1 - z} + \cdots$$

$$= \frac{1}{1 - z} + \frac{\Delta(z)}{1 - z}.$$

Hence from (III.8)

$$S(z) = \{(1 - z)^2 P(0, z)\}^{-1}. \quad \text{(III.10)}$$

The asymptotic properties of S_n as $n \to \infty$ can be inferred from the analytic behavior of $\Delta(z)$ as $z \to 1$ by employing the following Tauberian theorem[10]:

Let $A(y) = \sum a_n \exp(-ny)$ be convergent for all $y > 0$ and let $a_n > 0$ for all n. If as $y \to 0$

$$A(y) \sim \varphi(y^{-1}), \quad \text{(III.11a)}$$

where (i) $\varphi(x) = x^\sigma L(x)$ is a positive increasing function of x for x greater than some x_0, and which increases monotonically to infinity for x sufficiently large; (ii) σ is ≥ 0; and (iii) $L(cx) \sim L(x)$ as $x \to \infty$; then as $n \to \infty$

$$a_1 + a_2 + \cdots + a_n \sim \varphi(n)/\Gamma(\sigma + 1). \quad \text{(III.11b)}$$

In our problem we interpret $a_1 + \cdots + a_n$ as $\Delta_1 + \cdots + \Delta_n$ and $A(y)$ as $\Delta(e^{-y})$.

[10] G. H. Hardy, *Divergent Series* (Oxford University Press, New York, 1949).

As $z \to 1$ the asymptotic behavior of $P(0, z)$ in one, two, and three dimensions is as follows[2]:

$$\text{1D} \quad P(0, z) = (1 - z^2)^{-\frac{1}{2}}, \quad \text{(III.12a)}$$

$$\text{2D} \quad P(0, z) \sim -\pi^{-1} \log(1 - z), \quad \text{(III.12b)}$$

$$\text{3D} \quad P(0, z) \sim P(0, 1) + a(1 - z)^{\frac{1}{2}} + \cdots, \quad \text{(III.12c)}$$

where a is a constant which depends on the lattice. Then, if we let $z = \exp(-y)$ and let $y \to 0$,

$$\text{1D} \quad \Delta(z) \sim (2/y)^{\frac{1}{2}}, \quad \text{(III.13a)}$$

$$\text{2D} \quad \Delta(z) \sim (\pi/y)[1/\log(1/y)], \quad \text{(III.13b)}$$

$$\text{3D} \quad \Delta(z) \sim [yP(0, 1)]^{-1}. \quad \text{(III.13c)}$$

The Tauberian theorem given above applies directly to our problem[2] if we choose

$$\text{1D} \quad \sigma = \tfrac{1}{2}, \quad L(x) = 2^{\frac{1}{2}}, \quad \text{(III.14a)}$$

$$\text{2D} \quad \sigma = 1, \quad L(x) = \pi/\log x, \quad \text{(III.14b)}$$

$$\text{3D} \quad \sigma = 1, \quad L(x) = 1/P(0, 1). \quad \text{(III.14c)}$$

We therefore find for the number of distinct lattice points visited after n steps

$$\text{1D} \quad S_n \sim (8n/\pi)^{\frac{1}{2}}, \quad \text{(III.15a)}$$

$$\text{2D} \quad S_n \sim \pi n/\log n, \quad \text{(III.15b)}$$

$$\text{3D} \quad S_n \sim n/P(0, 1). \quad \text{(III.15c)}$$

These results have been derived by Erdos and Dvoretsky[3] and by Vineyard[4] by somewhat different methods. The values of $P(0, 1)$ are 1.5164 for a simple cubic lattice, 1.3445 for a face-centered and 1.3932 for a body-centered cubic lattice.[2,4]

It is interesting to note that the 2-D S_n/π has the same asymptotic behavior as the number of primes less than n. Perhaps one can find some deep connection between random walks on square lattices and the distribution of primes.

We have shown in Appendix C that the generating function for the average number of lattice points visited at least r times, $S_n^{(r)}$, is

$$S^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \frac{1}{(1 - z)^2 P(0, z)}, \quad \text{(III.16)}$$

while that of

$$\Delta_n^{(r)} = S_n^{(r)} - S_{n-1}^{(r)}$$

is

$$\Delta^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \frac{1}{(1 - z)P(0, z)}, \quad r \geq 2. \quad \text{(III.17)}$$

The average number of lattice points visited *exactly*

r times after n steps, $V_n^{(r)}$ is given by

$$V_n^{(r)} = S_n^{(r)} - S_n^{(r+1)}. \tag{III.18}$$

Its generating function is

$$V^{(r)}(z) = \sum_0^\infty V_n^{(r)} z^r$$

$$= \frac{1}{(1-z)^2[P(0,z)]^2}\left\{1 - \frac{1}{P(0,z)}\right\}^{r-1}. \tag{III.19}$$

By applying the above Tauberian theorem to Eq. (III.17) we can generalize (III.15c) to find $S_n^{(r)}$, the average number of points occupied at least r times in a walk of n steps on a three-dimensional lattice. If we set $z = e^{-y}$ and let $y \to 0$ we find

$$\Delta^{(r)}(e^{-y}) \sim \left\{1 - \frac{1}{P(0,1)}\right\}^{r-1} \frac{1}{P(0,1)y}, \tag{III.20}$$

so that in the notation of the Tauberian theorem $\sigma = 1$ and

$$L(x) = \frac{1}{P(0,1)}\left\{1 - \frac{1}{P(0,1)}\right\}^{r-1}$$

$$= \text{constant}. \tag{III.21}$$

Hence, since for $r > 1$

$$S_n^{(r)} = \Delta_1^{(r)} + \Delta_2^{(r)} + \cdots + \Delta_n^{(r)},$$

Eq. (III.16) implies that as $n \to \infty$

$$S_n^{(r)} \sim \frac{n}{P(0,1)}\left\{1 - \frac{1}{P(0,1)}\right\}^{r-1}. \tag{III.22}$$

Noting that the quantity $f = 1 - [P(0,1)]^{-1}$ is the probability that a random walker who starts from the origin ever returns to the origin, we can write

$$S_n^{(r)} \sim n(1-f)f^{r-1}. \tag{III.23}$$

The values of f for the three cubic lattices are sc 0.34056, bcc 0.28223, and fcc 0.25632.

As $n \to \infty$, the average number of points occupied on a 3-D lattice exactly r times in an n step walk is

$$V_n^{(r)} = S_n^{(r)} - S_n^{(r+1)} \sim n(1-f)^2 f^{r-1}. \tag{III.24}$$

If one wishes to find correction terms to the asymptotic formulas (III.15) for S_n, the number of points visited at least once in an n step walk, he must proceed in a more systematic manner. In the 3-D case it is shown in Appendix D that

$$P(0,z) = u_0 - u_1(1-z)^{\frac{1}{2}} + u_2(1-z) - u_3(1-z)^{\frac{3}{2}} + \cdots. \tag{III.25}$$

The numbers u_0 for the various cubic lattices are given in Eq. (D.3) of that appendix.[9] It was also shown that

$$u_1 = \begin{cases} (3/\pi)(\frac{3}{2})^{\frac{1}{2}} = 1.1695454 & \text{sc}, \quad \text{(III.26a)} \\ 1/2^{\frac{1}{2}}\pi = 0.2250791 & \text{bcc}, \quad \text{(III.26b)} \\ 3^{\frac{1}{2}}/4\pi = 0.4134967 & \text{fcc}. \quad \text{(III.26c)} \end{cases}$$

The values of u_2 and u_3 have not been calculated for the bcc and fcc; however, for the sc lattice,[11]

$$u_2 = 1.384761, \tag{III.27a}$$

$$u_3 = \frac{9}{4\pi}\left(\frac{3}{2}\right)^{\frac{1}{2}} = 0.877159. \tag{III.27b}$$

Equation (III.25) can be substituted into the generating function $S(z)$ [see Eq. (III.10)] to obtain

$$S(z) = [u_0(1-z)^2]^{-1} + (u_1/u_0^2)(1-z)^{-\frac{3}{2}} + [(u_1^2 - u_2u_0)/u_0^3](1-z)^{-1} + [(u_1^3 - 2u_0u_1u_2 + u_3u_0^2)/u_0^4](1-z)^{-\frac{1}{2}} + \cdots. \tag{III.28}$$

Now the coefficient of z^n in the series expansion of $(1-z)^m$ is

$$\text{for } m = -2\text{:} \quad (n+1), \tag{III.29a}$$

$$\text{for } m = -\tfrac{3}{2}\text{:} \quad (2n+1)!/2^{2n}n!\,n!, \tag{III.29b}$$

$$\text{for } m = -1\text{:} \quad 1, \tag{III.29c}$$

$$\text{for } m = -\tfrac{1}{2}\text{:} \quad (2n-1)!/2^{2n-1}n!\,(n-1)!. \tag{III.29d}$$

One can use Stirling's expansion for large n to find

$$\frac{(2n+1)!}{2^{2n}n!\,n!} \sim 2\left(\frac{n}{\pi}\right)^{\frac{1}{2}} \times \left[1 + \frac{3}{8n} - \frac{7}{128n^2} + \cdots\right], \tag{III.30a}$$

$$\frac{(2n-1)!}{2^{2n-1}n!\,(n-1)!} \sim \frac{1}{(n\pi)^{\frac{1}{2}}} \times \left[1 - \frac{1}{8n} + \frac{1}{128n^2} - \cdots\right]. \tag{III.30b}$$

Then

$$S_n \sim \frac{n}{u_0} + \frac{2u_1}{u_0^2}\left(\frac{n}{\pi}\right)^{\frac{1}{2}} + (u_1^2 - u_2u_0 + u_0^2)/u_0^3 + (3u_1u_0^2 + 4u_1^3 - 8u_0u_1u_2 + 4u_3u_0^2)/[4u_0^4(\pi n)^{\frac{1}{2}}] + O(1/n). \tag{III.31}$$

In the case of the bcc lattice

$$S_n \sim \frac{4\pi^3 n}{[\Gamma(\frac{1}{4})]^4} + \frac{16\pi^5}{[\Gamma(\frac{1}{4})]^8}\left(\frac{2n}{\pi}\right)^{\frac{1}{2}} + O(1)$$

$$= 0.71777001n + 0.130846n^{\frac{1}{2}} + O(1). \tag{III.32}$$

[11] A. Maradudin, E. Montroll, G. Weiss, R. Herman, and H. Milnes, "Green's Functions for Monatomic Simple Cubic Lattices," Acad. Roy. Belg. Cl. Sci. Mem. Coll. in 4° (2) 14 (1960) No. 7.

In the case of the fcc lattice

$$S_n \sim \frac{2^{11/3}n\pi^4}{9\{\Gamma(\frac{1}{3})\}^6} + \frac{2^{19/3}\pi^7}{9\{\Gamma(\frac{1}{3})\}^{12}}\left(\frac{n}{3\pi}\right)^{1/2} + O(1)$$

$$= 0.74368182n + 0.258048n^{1/2} + O(1), \quad \text{(III.33)}$$

while with the extra information available for the sc lattice one finds in that case

$$S_n \sim 0.65946267n + 0.573921n^{1/2}$$

$$+ 0.449530 + 0.40732n^{-1/2} + \cdots . \quad \text{(III.34)}$$

A similar expression can be obtained for the number of points occupied at least once after n steps on a 1-D lattice walk in which the walker steps only to a nearest-neighbor point on each step (steps in either direction being equally probable). Then from (III.10)

$$S(z) = \frac{(1-z^2)^{\frac{1}{2}}}{(1-z)^2} = \frac{[2-(1-z)]^{\frac{1}{2}}}{(1-z)^{\frac{1}{2}}}$$

$$= 2^{\frac{1}{2}}\{(1-z)^{-\frac{1}{2}} - \tfrac{1}{4}(1-z)^{-\frac{1}{2}}$$

$$- \tfrac{1}{32}(1-z)^{\frac{1}{2}} - \tfrac{1}{128}(1-z)^{\frac{3}{2}} - \cdots\}, \quad \text{(III.35)}$$

so that

$$S_n \sim \frac{2^{\frac{1}{2}}(2n+1)!}{2^{2n}n!\,n!}\left\{1 - \frac{1}{4(2n+1)}\right.$$

$$\left. - \frac{1}{32(4n^2-1)} - \cdots\right\}. \quad \text{(III.36)}$$

If n is chosen to be as small as 4 this yields 3.347 as compared with the exact value 3.375 given in Table II. By using Stirling's approximation [see Eq. (III.30)] for the factorials we find the somewhat simplified expression

$$S_n \sim \left(\frac{8n}{\pi}\right)^{\frac{1}{2}}\left\{1 + \frac{1}{4n} - \frac{3}{64n^2} + \cdots\right\}. \quad \text{(III.37)}$$

The generating function for the number of points which are occupied exactly once in an n step 1-D walk is, from (III.19) and (III.12a)

$$V^{(1)}(z) = [(1-z)P(z,0)]^{-2}$$

$$= (1-z^2)/(1-z)^2 = (1+z)/(1-z)$$

$$= 1 + 2z + 2z^2 + 2z^3 + \cdots . \quad \text{(III.38)}$$

Hence

$$V_1^{(1)} = 1 \quad \text{and} \quad V_n^{(1)} = 2 \quad \text{for} \quad n > 1. \quad \text{(III.39)}$$

The asymptotic expression for $V_n^{(1)}$ for large n on a 2-D square lattice can be obtained by finding the generating function for

$$D_n^{(1)} = V_n^{(1)} - V_{n-1}^{(1)},$$
$$D^{(1)}(z) = -1 + (1-z)^{-1}[P(z,0)]^2 \quad \text{(III.40)}$$

(here $D_n^{(1)}$ is analogous to Δ_n in the calculation of S_n). By employing (III.40) and our Tauberian theorem we find

$$V_n^{(1)} \sim n\pi^2/(\log n)^2 \quad \text{(III.41)}$$

to be the asymptotic number of points occupied exactly once in the 2-D case. The result has also been derived by Erdos and Taylor[5] by a different method.

The 1-D generating function for $S_n^{(2)}$, the number of points occupied at least twice in an n-step walk is

$$S^{(2)}(z) \equiv \{1 - (1-z^2)^{\frac{1}{2}}\}\frac{(1-z^2)^{\frac{1}{2}}}{(1-z)^2}$$

$$= S^{(1)}(z) - \left(\frac{1+z}{1-z}\right). \quad \text{(III.42a)}$$

Hence when $n \geq 2$

$$S_n^{(2)} = S_n^{(1)} - 2, \quad \text{(III.42b)}$$

which can be verified in Table II. Similarly,

$$S^{(3)}(z)$$
$$= [1 - 2(1-z^2)^{\frac{1}{2}} + (1-z^2)](1-z^2)^{\frac{1}{2}}/(1-z)^2$$
$$= (2-z^2)S^{(1)}(z) - 2(1+z)/(1-z)$$

Hence

$$S_n^{(3)} = 2S_n^{(1)} - S_{n-2}^{(1)} - 4 \quad \text{if} \quad n \geq 4. \quad \text{(III.42c)}$$

TABLE I. Values of $P(\mathbf{s}, 1)$ for a simple cubic lattice when $s^2 = s_1^2 + s_2^2 + s_3^2 < 15$. These numbers correspond to the symmetrical case with $P(s_1s_2s_3, 1) = P(s_2s_1s_3, 1) = \cdots$, etc. This function is the lattice Green's function defined by (II.6) and (I.5) when $z = 1$.

(s_1, s_2, s_3)	$P(\mathbf{s}, 1)$	(s_1, s_2, s_3)	$P(\mathbf{s}, 1)$
001	0.516387	023	0.132451
002	0.257336	111	0.261470
003	0.165271	112	0.191792
011	0.331149	113	0.144196
012	0.215590	122	0.156953
013	0.153139	123	0.126946
022	0.168331	222	0.135908

TABLE II. $S_n^{(r)}$ = Average number of points occupied at least r times in a 1-D walk of n steps.

n/r	1	2	2	4	5
0	1	0	0	0	0
1	2	0	0	0	0
2	5/2	1/2	0	0	0
3	3	1	0	0	0
4	27/8	11/8	1/4	0	0
5	15/4	7/4	1/2	0	0
6	65/16	33/16	3/4	1/8	0
7	35/8	19/8	1	1/4	0

TABLE III. $V_n^{(r)}$ = Average number of points occupied exactly r times in a 1-D walk of n steps.

n/r	1	2	3	4	5
0	1	0	0	0	0
1	2	0	0	0	0
2	2	1/2	0	0	0
3	2	1	0	0	0
4	2	9/8	1/4	0	0
5	2	5/4	1/2	0	0
6	2	21/16	5/8	1/8	0
7	2	11/8	3/4	1/4	0

Similarly

$$S_n^{(4)} = 4S_n^{(1)} - 3S_{n-2}^{(1)} - 6 \quad \text{if} \quad n \geq 6, \qquad \text{(III.42d)}$$

etc.

This scheme can be continued further and when these formulas are combined with (III.36) and (III.37), very accurate asymptotic expansions can be found for $S_n^{(r)}$ for 1-D walks, $r \ll n$.

IV. THE NUMBER OF VISITS TO A GIVEN LATTICE POINT DURING A WALK OF n STEPS

The probability that a point s is visited at least r times in an n-step walk is

$$\sum_{i=1}^{n} F_i^{(r)}(s) \quad \text{if} \quad \mathbf{s} \neq 0,$$

$$\sum_{i=1}^{n} F_i^{(r-1)}(0) \quad \text{if} \quad s = 0,$$

so that the probability that s is visited *exactly* r times is

$$\beta_n^{(r)}(\mathbf{s}) = \begin{cases} \sum_{i=1}^{n} [F_i^{(r)}(\mathbf{s}) - F_i^{(r+1)}(\mathbf{s})], \\ \qquad\qquad \text{if} \quad \mathbf{s} \neq 0, \\ \sum_{i=1}^{n} [F_i^{(r-1)}(0) - F_i^{(r)}(0)], \\ \qquad\qquad \text{if} \quad \mathbf{s} = 0. \end{cases} \qquad \text{(IV.1)}$$

The formulas for $\beta_n^{(r)}(0)$ are distinctive because the walker starts at the origin.

The generating function for $\beta^{(r)}(\mathbf{s}, z)$,

$$\beta^{(r)}(\mathbf{s}, z) \equiv \sum_{1}^{n} z^n \beta_n^{(r)}, \qquad \text{(IV.2)}$$

is easily seen from (I.20) to be

$$\beta^{(r)}(\mathbf{s}, z) = \begin{cases} (1-z)^{-1} F(\mathbf{s}, z)[1 - F(0, z)] \\ \qquad \times [F(0, z)]^{r-1}, \ \mathbf{s} \neq 0, \\ (1-z)[F(0, z)]^{r-1} \\ \qquad \times [1 - F(0, z)], \ \mathbf{s} = 0. \end{cases} \qquad \text{(IV.3)}$$

The mean number of times the point s has been visited after n steps is

$$M_n(\mathbf{s}) = \sum r\beta_n^{(r)}(\mathbf{s}). \qquad \text{(IV.4)}$$

This has the generating function

$$M(\mathbf{s}, z) = \sum_{r=1}^{\infty} \sum_{n=1}^{\infty} r\beta_n^{(r)}(\mathbf{s}) z^n$$

$$= \sum_{r=1}^{\infty} r\beta^{(r)}(\mathbf{s}, z)$$

$$= \frac{F(\mathbf{s}, z)}{(1-z)[1 - F(0, z)]} \quad \text{if} \quad \mathbf{s} \neq 0$$

$$= (1-z)^{-1} P(\mathbf{s}, z). \qquad \text{(IV.5)}$$

If $\mathbf{s} = 0$,

$$M(0, z) = \{(1-z)[1 - F(0, z)]\}^{-1}$$

$$= (1-z)^{-1} P(0, z). \qquad \text{(IV.6)}$$

Hence (IV.5) is valid for all s including $\mathbf{s} = 0$.

The asymptotic form for $M_n(0)$ for 3-D lattices can be obtained by using the expression for $P(0, z)$ given in Appendix F. There it is shown that

$$P(0, z) \sim u_0 - [2(1-z)]^{\frac{1}{2}}/\pi\sigma_1\sigma_2\sigma_3 + \cdots, \qquad \text{(IV.7)}$$

where the u_0 and σ's are defined generally and evaluated for walks on cubic lattices where only steps to nearest-neighbor points (all with equal probability) are taken. By combining Eqs. (IV.6), (IV.7), and (III.29) we obtain

$$M_n(0) \sim u_0 - (2/\pi n)^{\frac{1}{2}}/\pi\sigma_1\sigma_2\sigma_3 + O(1/n). \qquad \text{(IV.8)}$$

The numerical results are

$$M_n(0) \sim \begin{cases} 1.51639 - 1.31969n^{-\frac{1}{2}} + \cdots & \text{sc}, \\ 1.39320 - 0.25397n^{-\frac{1}{2}} + \cdots & \text{fcc}, \\ 1.34466 - 0.46658n^{-\frac{1}{2}} + \cdots & \text{bcc}. \end{cases} \qquad \text{(IV.9)}$$

As $n \to \infty$

$$M_n(\mathbf{s}) \to P(\mathbf{s}, 1). \qquad \text{(IV.10)}$$

These functions have been tabulated for[11] sc lattices when $s^2 < 25$. Some values are given in Table I.

When s is large and $z \to 1$ we have from (I.18b) [where $\lambda^2 = \sum (s_i/\sigma_i)^2$]

$$P(\mathbf{s}, z) \sim \frac{\exp\{-\lambda[2(1-z)^{\frac{1}{2}}]\}}{\lambda\sigma_1\sigma_2\sigma_3(2\pi)^2}$$

$$\sim \frac{1}{\lambda\sigma_1\sigma_2\sigma_3(2\pi)^2}\{1 - \lambda[2(1-z)]^{\frac{1}{2}} + \cdots\}. \qquad \text{(IV.11)}$$

Hence, from (IV.5), (IV.7), and (III.29), when s

and n are both large, but still with $s \ll n^{\frac{1}{2}}$,

$$M_n(\mathbf{s}) \sim \frac{1}{\lambda\sigma_1\sigma_2\sigma_3(2\pi)^2} \times \left\{1 - \lambda\left(\frac{2}{\pi n}\right)^{\frac{1}{2}} + \cdots\right\}. \quad \text{(IV.12)}$$

Employing the σ values given in Appendix D for the walks involving only steps to nearest-neighbor lattice points on cubic lattices we find

$$M_n(\mathbf{s}) \sim \begin{cases} \frac{3}{4s\pi^2}\left[1 - s\left(\frac{6}{\pi n}\right)^{\frac{1}{2}} + \cdots\right] & \text{sc} \\ \frac{1}{4s\pi^2}\left[1 - s\left(\frac{2}{\pi n}\right)^{\frac{1}{2}} + \cdots\right] & \text{bcc} \\ \frac{3}{8s\pi^2}\left[1 - s\left(\frac{3}{\pi n}\right)^{\frac{1}{2}} + \cdots\right] & \text{fcc.} \end{cases} \quad \text{(IV.13)}$$

A word of caution should be given concerning these results. One would expect that $M_n(\mathbf{s})$ should appear with some ordering with respect to nearest neighbors. However the bcc results are not between the sc and fcc. This is because all lattices were obtained by restricting walks on a fundamental sc lattice. If the unit cells of each of the lattices were made the same size and s reexpressed as a length the results would fall properly in order.

V. LATTICE WALKS FOR CONTINUOUS TIME VARIABLE

The preceding results can be used as a basis for the analysis of continuous time random walks on discrete lattices. In this theory we shall be interested in functions like $\bar{P}(\mathbf{s}, t)$ and $\bar{F}(\mathbf{s}, t)$ (the probability of being at $\mathbf{s}$ at time t) and the probability density for reaching $\mathbf{s}$ for the first time at time t, respectively. We shall assume that jumps are made at random times $t_1, t_2, t_3, \cdots$ where the random variables

$$T_1 = t_1, \quad T_2 = t_2 - t_1, \cdots, \quad T_n = t_n - t_{n-1}, \cdots \quad \text{(V.1)}$$

have a common density $\psi(t)$. It will be convenient to define a further class of probability densities $\{\psi_n(t)\}$ by

$$\psi_0(t) = \delta(t), \quad \text{(V.2)}$$

$$\psi_n(t) = \int_0^t \psi(\tau)\psi_{n-1}(t - \tau)\, d\tau, \quad n = 1, 2, 3, \cdots. \quad \text{(V.3)}$$

These are the probability densities for the occurrence of the nth step at time t. The most significant property of the $\psi_n(t)$ is the fact that their Laplace transforms are

$$\int_0^\infty e^{-ut}\psi_n(t)\, dt = [\psi^*(u)]^n, \quad \text{(V.4)}$$

where

$$\psi^*(u) = \int_0^\infty e^{-ut}\psi(t)\, dt. \quad \text{(V.5)}$$

In terms of the $F_n(\mathbf{s})$ defined in Sec. 1, $\bar{F}(\mathbf{s}, t)$ is given by

$$\bar{F}(\mathbf{s}, t) = \sum_{n=0}^\infty F_n(\mathbf{s})\psi_n(t) \quad \text{(V.6)}$$

and its Laplace transform is

$$\bar{F}^*(\mathbf{s}, u) = \int_0^\infty \bar{F}(\mathbf{s}, t)e^{-ut}\, dt = \sum_{n=0}^\infty F_n(\mathbf{s})[\psi^*(u)]^n = F[\mathbf{s}, \psi^*(u)], \quad \text{(V.7)}$$

where $F(\mathbf{s}, z)$ is the generating function of Eq. (I.17).

The function $\bar{P}(\mathbf{s}, t)$ is almost as simply related to the generating function $P(\mathbf{s}, z)$. Let $Q(\mathbf{s}, t)$ be the probability density for the random walk to reach $\mathbf{s}$ at time t (not necessarily for the first time) and let

$\Psi(t)$ = probability that walker remains fixed in time interval $(0, t)$

$$= 1 - \int_0^t \psi(x)\, dx = \int_t^\infty \psi(x)\, dx. \quad \text{(V.8)}$$

Then

$$\bar{P}(\mathbf{s}, t) = \int_0^t Q(\mathbf{s}, \tau)\Psi(t - \tau)\, d\tau, \quad \text{(V.9)}$$

or, in terms of Laplace transforms,

$$\bar{P}^*(\mathbf{s}, u) = Q^*(\mathbf{s}, u)[1 - \psi^*(u)]/u. \quad \text{(V.10)}$$

But $Q(s, t)$ is given by

$$Q(\mathbf{s}, t) = \sum_{n=0}^\infty P_n(\mathbf{s})\psi_n(t) \quad \text{(V.11)}$$

or

$$Q^*(\mathbf{s}, u) = \sum_{n=0}^\infty P_n(\mathbf{s})[\psi^*(u)]^n = P[\mathbf{s}, \psi^*(u)], \quad \text{(V.12)}$$

so that only the generating functions already discussed need be calculated.

Moments for various quantities of interest are easily derived from the formulas above. For example the first moment and variance of the first-passage

time to s are

$$\bar{t} = -\frac{\partial F[\mathbf{s}, \psi^*(u)]}{\partial u}\Big]_{u=0+} = \langle n(\mathbf{s})\rangle \bar{T}, \qquad \text{(V.13a)}$$

$$\overline{t^2} - \bar{t}^2 = [\langle n^2(\mathbf{s})\rangle - \langle n(\mathbf{s})\rangle^2]\bar{T}^2 + \langle n(\mathbf{s})\rangle[\overline{T^2} - \bar{T}^2], \qquad \text{(V.13b)}$$

where $\overline{T^n}$ is the nth moment of the time between steps and $\langle n(s)\rangle$ and $\langle n^2(s)\rangle$ are given by (II.2) and (II.3).

Continuous analogues of other discrete results are obtained in the same manner. For example, the probability density for the random walker to reach s for the rth time is

$$\overline{F^{(r)}}(\mathbf{s}, t) = \sum_{n=0}^{\infty} F_n^{(r)}(\mathbf{s})\psi_n(t) \qquad \text{(V.14a)}$$

or

$$\overline{F^{(r)}}^*(\mathbf{s}, u) = F^{(r)}[\mathbf{s}, \psi^*(u)], \qquad \text{(V.14b)}$$

where $F^{(r)}(\mathbf{s}, z)$ is given by (I.20).

We can also consider the statistics of the number of distinct steps visited after a time t. Let $S(t)$ be the average number of lattice points visited at least once in time t. Then

$$S(t) = \sum_{s} \int_0^t F^{(r)}(\mathbf{s}, \tau)\, d\tau. \qquad \text{(V.15a)}$$

Hence the Laplace transform of $S(t)$ is

$$\mathfrak{L}\{S(t)\} = \frac{\psi^*(u)}{u[1 - \psi^*(u)]P(0, \psi^*(u))}. \qquad \text{(V.15b)}$$

To find the large t behavior of $S(t)$ it is necessary to use the expansion

$$\psi^*(u) = 1 - u\bar{T} + o(u) \qquad \text{(V.16)}$$

in Eq. (V.5), together with the asymptotic forms of Eq. (III.12) for the behavior of $P(0, z)$ in the neighbor hood of $z = 1$. In this way, we find that in one dimension

$$\mathfrak{L}\{S(t)\} = (2/\bar{T})^{\frac{1}{2}}u^{-\frac{3}{2}} + O(u^{-1}) \qquad \text{(V.17)}$$

in the neighborhood of $u = 0$. But, by a Tauberian theorem[7] this implies that

$$S(t) = (8t/\pi\bar{T})^{\frac{1}{2}} + O(1). \qquad \text{(V.18)}$$

In three dimensions the result is

$$S(t) = (t/\bar{T})/P(0, 1) + O(1). \qquad \text{(V.19)}$$

The results are in agreement with (III.15a) and (III.15b) since the number of steps n is just $t/\bar{T}$ in the case of steps at regular time intervals.

VI. EFFECT OF TRAPS ON PROBABILITY OF RETURN TO THE ORIGIN ON A 1-D LATTICE

Another type of random walk problem is concerned with effect of traps on the probability of a walker eventually returning to the origin. We shall limit ourselves here to a discussion of the 1-D case while an analysis of the 2-D and 3-D problems, which are much more difficult, will be given elsewhere.

It has been shown[2] that in the presence of one trap at l_1 and another at l_2 with $l_2 < 0 < l_1$ the probability that a walker initially at the origin is trapped before return to the origin is

$$(l_1 - l_2)/2l_1(-l_2) = \tfrac{1}{2}(l_1^{-1} - l_2^{-1}).$$

This probability is not changed by the addition of any number of new traps *which are not located in the interval* $l_2 < 0 < l_1$.

Let c be the concentration of independently located traps. Then, if it is known that the origin is not a trap, the probability that a trap exists at l_1 and at l_2 and none in between is

$$c(1 - c)^{-l_2-1}(1 - c)^{l_1-1}c.$$

Hence the probability of our walker being trapped before returning to the origin is

$$\sum_{l_1=1}^{\infty} \sum_{l_2=-1}^{-\infty} c^2(1 - c)^{l_1-l_2-2}(\tfrac{1}{2})(l_1^{-1} - l_2^{-1}) = c^2(1 - c)^{-1}\left\{\sum_{l=1}^{\infty}(1 - c)^{l-1}\right\}\left\{\sum_{l_1=1}^{\infty}(1 - c)^{l_1}/l_1\right\} = -[c/(1 - c)]\log c.$$

Then as a function of concentration of traps, the probability of a walker returning to the origin before being trapped is

$$F(c) = 1 + [c/(1 - c)]\log c.$$

APPENDIX A. ASYMPTOTIC FORM OF $\varphi(s, z)$ AS $s \to \infty$

The Green's function

$$\varphi(\mathbf{s}, z) = \frac{1}{(2\pi)^k}\int_{-\pi}^{\pi}\cdots\int \frac{\exp i\mathbf{s}\cdot\boldsymbol{\vartheta}\, d^k\boldsymbol{\vartheta}}{1 - z\lambda(\boldsymbol{\vartheta})} \qquad \text{(A.1)}$$

can be expressed as

$$\varphi(\mathbf{s}, z) = \frac{1}{(2\pi)^k}\int_0^{\infty} e^{-\alpha}\, d\alpha \int_{-\pi}^{\pi}\cdots\int e^{i\mathbf{s}\cdot\boldsymbol{\vartheta}} \times e^{\alpha z\lambda(\boldsymbol{\vartheta})}\, d^k\boldsymbol{\vartheta}. \qquad \text{(A.2)}$$

When s is very large the main contribution to the $\boldsymbol{\vartheta}$ integration comes from small values of $|\boldsymbol{\vartheta}|$. In this

range in a symmetrical random walk (see I.4)

$$\lambda(\boldsymbol{\vartheta}) = 1 - \tfrac{1}{2}\sum \sigma_i^2\vartheta_i^2 + \tfrac{1}{4}\sum_{ij}{}' \mu_{ij}\vartheta_i^2\vartheta_j^2 - \cdots . \quad \text{(A.3)}$$

If we let $s_i\vartheta_i = \varphi_i$ and $\lambda_i = s_i/\sigma_i$, then $\varphi(s, z)$ becomes

$$\varphi(s, z) = \frac{1}{(2\pi)^k}\int_0^\infty e^{-\alpha(1-z)}\, d\alpha$$
$$\times \int_{-\pi s_1}^{\pi s_1}\cdots\int_{-\pi s_k}^{\pi s_k} e^{i(\varphi_1+\varphi_2+\cdots)}e^{-\frac{1}{2}\alpha z\sum \lambda_i^{-2}\varphi_i^2}$$
$$\times \{1 + \tfrac{1}{4}\alpha z\sum (\mu_{ij}/s_i^2s_j^2)\varphi_i^2\varphi_j^2 + \cdots\}\, d^k\varphi/s_1\cdots s_k. \quad \text{(A.4)}$$

As all $s_i \to \infty$ the limits on the φ integration can be extended to $\pm\infty$ with errors of only $O[\exp(-cs_i^2)]$ appearing.

If we let

$$R_n(a) = \int_{-\infty}^{\infty} e^{i\varphi}e^{-\frac{1}{2}a\varphi^2}\varphi^n\, d\varphi, \quad \text{(A.5)}$$

then

$$\varphi(s, z) \sim (2\pi)^{-k}\int_0^\infty e^{-\alpha(1-z)}\, d\alpha\left\{\prod_{\nu=1}^k R_0(\alpha z\lambda_\nu^{-2})\right\}$$
$$\times\left\{1 + \tfrac{1}{4}\alpha z\sum_{i=1}^k (\mu_{ii}/s_i^4)(R_4/R_0)_{\alpha z\lambda_i^{-2}}\right.$$
$$\left. + \tfrac{1}{4}\alpha z\sum_{ij}{}' \frac{\mu_{ij}}{s_i^2s_j^2}\left(\frac{R_2}{R_0}\right)_{\alpha z\lambda_i^{-2}}\left(\frac{R_2}{R_0}\right)_{\alpha z\lambda_j^{-2}} + \cdots\right\},$$

where as usual the prime in the summation indicates that the terms with $i = j$ are to be omitted.

From standard integral tables one finds

$$R_0(a) = (2\pi/a)^{\frac{1}{2}}\exp(-1/2a),$$
$$(R_2/R_0)_a = a^{-1}(1 - a^{-1}),$$
$$(R_4/R_0)_a = a^{-2}(3 - 6a^{-1} + a^{-2}).$$

Then, if we let

$$S_n(z) = \int_0^\infty \alpha^{-\frac{1}{2}n}e^{-\alpha(1-z)}\exp\left(-\frac{1}{2\alpha z}\sum \lambda_\nu^2\right) d\alpha,$$

we find

$$\varphi(\mathbf{s}, z) \sim \frac{(2\pi z)^{-\frac{1}{2}k}}{\sigma_1\cdots\sigma_k}\left[S_k + \sum_{i=1}^k \frac{\mu_{ii}}{4z\sigma_i^4}\right.$$
$$\times (3S_{k+2} - 6z^{-1}\lambda_i^2S_{k+4} + z^{-2}\lambda_i^4S_{k+6})$$
$$+ \tfrac{1}{4}\sum_{ij}{}' \frac{\mu_{ij}}{z\sigma_i^2\sigma_j^2}[S_{k+2} - z^{-1}(\lambda_i^2 + \lambda_j^2)S_{k+4}$$
$$\left. + z^{-2}\lambda_i^2\lambda_j^2S_{k+6}] + \cdots\right].$$

In the special case $z = 1$, we see that

$$S_n(1) = (2/\lambda^2)^{\frac{1}{2}(n-2)}\Gamma(\tfrac{1}{2}n - 1)$$

where

$$\lambda^2 = \sum \lambda_\nu^2 = \sum_{\nu=1}^k s_\nu^2/\sigma_\nu^2.$$

Generally,

$$S_n(z) = 2\left(\frac{2}{\lambda}\right)^{\frac{1}{2}n-1}[z(1-z)]^{\frac{1}{4}(n-2)}K_{\frac{1}{2}n-1}\left(\left[\frac{\lambda^2}{z}(1-z)\right]^{\frac{1}{2}}\right)$$

where K_ν is the νth modified Bessel Function of the second kind. When $z = 1$

$$\varphi(\mathbf{s}, 1) = \frac{\Gamma(\frac{1}{2}k - 1)}{2\sigma_1\cdots\sigma_k\pi^{\frac{1}{2}k}\lambda^{k-2}}\left\{1 - \frac{(1 - \frac{1}{2}k)}{2\lambda^2}\sum_{i=1}^k \frac{\mu_{ii}}{\sigma_i^2}\right.$$
$$\times\left[3 - 6k\left(\frac{\lambda_i}{\lambda}\right)^2 + k(k+2)\left(\frac{\lambda_i}{\lambda}\right)^4\right]$$
$$- (1/2\lambda^2)(1 - \tfrac{1}{2}k)\sum_{ij}{}' \frac{\mu_{ij}}{\sigma_i^2\sigma_j^2}[1 - k(\lambda_i^2 + \lambda_j^2)/2\lambda^2$$
$$\left. + k(k+2)\lambda_i^2\lambda_j^2/\lambda^4] + O(\lambda^{-4})\right\}.$$

If $\varphi_1(\mathbf{s}, z)$ is defined [see Eq. (I.9)] as

$$\varphi_1(\mathbf{s}, z) = \frac{1}{(2\pi)^k}\int_{-\pi}^{\pi}\cdots\int \frac{\exp(i\boldsymbol{\vartheta}\cdot\mathbf{s})\, d^k\boldsymbol{\vartheta}}{1 - z + \frac{1}{2}z(\sigma_1^2\vartheta_1^2 + \cdots + \sigma_k^2\vartheta_k^2)},$$

then as $\mathbf{s} \to \infty$ and $z \to 1$ when $k \geq 3$, then [see Eq. (I.186)]

$$\varphi_1(\mathbf{s}, z) \sim \frac{\Gamma(\frac{1}{2}k - 1)}{2\sigma_1\cdots\sigma_k\pi^{\frac{1}{2}k}\lambda^{k-2}},$$

which is the leading term in $\varphi(\mathbf{s}, 1)$. Hence if we let

$$\varphi(\mathbf{s}, z) = \varphi_1(\mathbf{s}, z) + \varphi_2(\mathbf{s}, z)$$

where $\varphi_2(s, z)$ is defined as $\varphi(\mathbf{s}, z) - \varphi_1(\mathbf{s}, z)$, we see that when $k \geq 3$

$$\lim_{\mathbf{s}\to\infty}\frac{\varphi_1(\mathbf{s}, 1)}{\varphi_2(\mathbf{s}, 1)} = 0.$$

APPENDIX B. CALCULATION OF 2-D $\varphi(0, 1)$ FOR $N \times N$ LATTICE AS $N \to \infty$

The expression for $\varphi(0, 1)$ in a finite lattice is (Eq. I.16)

$$\varphi(0, 1) = N^{-2}\sum_{r_1=1}^{N-1}\sum_{r_2=1}^{N-1}\left\{1 - \lambda\left(\frac{2\pi r}{N}\right)\right\}^{-1}$$
$$= 4N^{-2}\sum_{1}^{[(N-1)/2]}\sum_{1}^{[(N-1)/2]}\{1 - \lambda\}^{-1}$$
$$+ O(1/N). \quad \text{(B.1)}$$

As $N \to \infty$ this sum approaches a divergent integral, the divergence being related to the smallness of $1 - \lambda(2\pi r/N)$ as $(2\pi r/N) \to 0$. Hence one would

expect the main contribution to (0, 1) to result from small integral values of r_1 and r_2. In this range one can approximate λ by [see Eq. (I.4)]

$$\lambda(2\pi\mathfrak{r}/N) \sim 1 - (2\pi^2/N^2)(\sigma_1^2 r_1^2 + \sigma_2^2 r_2^2) + \cdots . \quad \text{(B.2)}$$

We now restrict ourselves to $\sigma_1 = \sigma_2$, the more general case being amenable to a similar analysis.

The range of summation in (B.1) is divided into two parts; the first part containing those lattice points (r_1, r_2) such that $(r_1^2 + r_2^2)^{\frac{1}{2}} < \alpha N$ where α is small enough so that (B.2) is a good approximation of λ for all these points, and the second containing the remainder of the lattice points. It can be shown that the contribution of the second set to $\varphi(0, 1)$ remains bounded as $N \to \infty$. The contribution of the first set is

$$4N^{-2} \sum_{1<(r_1^2+r_2^2)^{\frac{1}{2}}<\alpha N} \sum (N^2/2\pi^2\sigma_1^2)(r_1^2 + r_2^2)^{-1}.$$

When N is sufficiently large, the sum is well approximated by the corresponding integral, which we express in polar coordinates

$$\sum_{1<(r_1^2+r_2^2)^{\frac{1}{2}}<\alpha N} (r_1^2 + r_2^2)^{-1} \sim \int_1^{\alpha N} \frac{2\pi j\, dj}{j^2} = \frac{\pi}{2} \log \alpha N.$$

Hence, as $N \to \infty$ for fixed α,

$$\varphi(0, 1) \sim (1/\pi\sigma_1^2) \log N.$$

In the unsymmetric case $\sigma_1 \neq \sigma_2$, one finds

$$\varphi(0, 1) \sim (1/\pi\sigma_1\sigma_2) \log N.$$

The above ideas can, with a little effort, be made completely rigorous.

APPENDIX C. GENERATING FUNCTION FOR AVERAGE NUMBER OF POINTS VISITED AT LEAST r TIMES IN AN n-STEP WALK

Let $S_n^{(r)}$ be the average number of lattice points visited at least r times in an n-step walk. Then

$$S_n^{(r)} = F_1^{(r-1)}(0) + \cdots + F_n^{(r-1)}(0) + \sum_{\mathbf{s}}{}' \{F_1^{(r)}(\mathbf{s}) + F_2^{(r)}(\mathbf{s}) + \cdots + F_n^{(r)}(\mathbf{s})\}, \quad \text{(C.1)}$$

where the primed summation proceeds over all lattice points except the origin. As usual $F_j^{(r)}(\mathbf{s})$ is the probability that the walker arrives at $\mathbf{s}$ for the rth time on the jth step. The sum

$$F_1^{(r)}(s) + F_2^{(r)}(s) + \cdots + F_n^{(r)}(s)$$

represents the probability that the point $\mathbf{s}$ has been occupied *at least* r times in n steps. The reason

$$F_1^{(r-1)}(0) + \cdots + F_n^{(r-1)}(0)$$

is chosen to represent $(r - 1)$ returns to the origin instead of r is that the walker started at the origin, so visiting the origin r times means *returning* to it $r - 1$ times.

It is convenient to define a quantity

$$\Delta_k^{(r)} = S_k^{(r)} - S_{k-1}^{(r)}. \quad \text{(C.2)}$$

Since $S_0^{(1)} = 1$ and $S_1^{(1)} = 2$ while $S_0^{(r)} = S_1^{(r)} = 0$ for $r > 1$,

$$\Delta_1^{(1)} = 1 \quad \text{and} \quad \Delta_1^{(r)} = 0 \quad \text{if} \quad r > 1. \quad \text{(C.3)}$$

Also

$$S_n^{(r)} = \delta_{r,1} + \Delta_1^{(r)} + \Delta_2^{(r)} + \cdots + \Delta_n^{(r)}. \quad \text{(C.4)}$$

Through the use of an appropriate Tauberian Theorem we will be able to find the asymptotic properties of $S_n^{(r)}$ in terms of the properties of the generating function

$$\Delta^{(r)}(z) = \sum_{n=1}^{\infty} z^n \Delta_n^{(r)}. \quad \text{(C.5)}$$

Note that

$$\Delta_n^{(r)} = F_n^{(r-1)}(0) + \sum_{\mathbf{s}}{}' F_n^{(r)}(\mathbf{s}) = [F_n^{(r-1)}(0) - F_n^{(r)}(0)] + \sum_{\mathbf{s}} F_n^{(r)}(\mathbf{s}). \quad \text{(C.6)}$$

Hence if we multiply this equation by z^n and sum from $n = 1$ to ∞ we find

$$\Delta^{(r)}(z) = \{F^{(r-1)}(0, z) - F^{(r)}(0, z)\} + \sum_{\mathbf{s}} F^{(r)}(\mathbf{s}, z).$$

From Eq. (I.20) we obtain

$$\Delta^{(r)}(z) = \{F(0, z)\}^{r-1}\{1 - F(0, z) + \sum_{\mathbf{s}} F(\mathbf{s}, z)\},$$

while Eq. (I.18) implies

$$\Delta^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \times \left\{\frac{1}{P(0, z)} + \sum_{\mathbf{s}} \left[\frac{P(\mathbf{s}, z) - \delta_{\mathbf{s},0}}{P(0, z)}\right]\right\}.$$

Finally from (I.14b)

$$\Delta^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \{(1 - z)P(0, z)\}^{-1}.$$

From this expression and (C.4) one finds

$$S^{(r)}(z) = \left\{1 - \frac{1}{P(0, z)}\right\}^{r-1} \{(1 - z)^2 P(0, z)\}^{-1}. \quad \text{(C.7)}$$

APPENDIX D. THE ASYMPTOTIC FORM OF $P(0, z)$ AS $z \to 1$ FOR 3-D LATTICES

The generating function

$$P(0, z) = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} \frac{d^3\varphi}{1 - z\lambda(\varphi)} \quad \text{(D.1)}$$

can be expressed as

$$\frac{1}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{d^3\varphi}{1-\lambda(\varphi)}$$

$$-\frac{(1-z)}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{\lambda(\varphi)\,d^3\varphi}{[1-\lambda(\varphi)][1-z\lambda(\varphi)]}=u_0-\delta. \quad \text{(D.2)}$$

The first part, u_0 has been found by G. N. Watson[9] for simple, body-centered, and face-centered cubic lattices. His results are

$$\begin{aligned} &\text{sc} \quad 1.5163860591,\\ &\text{bcc} \quad (4\pi^3)^{-1}[\Gamma(\tfrac{1}{4})]^4 = 1.3932039297, \quad \text{(D.3)}\\ &\text{fcc} \quad 9\{\Gamma(\tfrac{1}{3})\}^6 2^{-11/3}\pi^{-4} = 1.3446610732. \end{aligned}$$

We shall be concerned with the determination of δ as $z \to 1$.

The main contribution to δ as $z \to 1$ comes from values of φ close to the origin. We can write

$$\lambda(\varphi) = 1 - \tfrac{1}{2}(\sigma_1^2\varphi_1^2 + \sigma_2^2\varphi_2^2 + \sigma_3^2\varphi_3^2) + O(\varphi^4). \quad \text{(D.4)}$$

For example in the case of steps to the nearest-neighbor lattice points only on cubic lattices one finds from (I.5) that

$$\begin{aligned} &\text{sc} \quad \sigma_1 = \sigma_2 = \sigma_3 = (\tfrac{1}{3})^{\frac{1}{2}}, \quad \text{(D.5a)}\\ &\text{bcc} \quad \sigma_1 = \sigma_2 = \sigma_3 = 1, \quad \text{(D.5b)}\\ &\text{fcc} \quad \sigma_1 = \sigma_2 = \sigma_3 = (\tfrac{2}{3})^{\frac{1}{2}}. \quad \text{(D.5c)} \end{aligned}$$

As $\varphi \to 0$ and $z \to 1$ the integrand of δ becomes

$$2/\{(\sigma_1^2\varphi_1^2 + \sigma_2^2\varphi_2^2 + \sigma_3^2\varphi_3^2) \times [(1-z) + \tfrac{1}{2}(\varphi_1^2\sigma_1^2 + \varphi_2^2\sigma_2^2 + \varphi_3^2\sigma_3^2) + \cdots]\}.$$

It can be shown that as $z \to 1$ the range of integration can be made infinite in δ if one is concerned only with terms first order in $(z-1)$. Then, if we let $x_i = \sigma_i\varphi_i$ and calculate δ using polar coordinates with $r^2 = x_1^2 + x_2^2 + x_3^2$ we find

$$\delta \sim \frac{1-z}{\sigma_1\sigma_2\sigma_3\pi^2}\int_0^\infty \frac{dr}{(1-z)+\frac{1}{2}r^2} = \frac{[\frac{1}{2}(1-z)]^{\frac{1}{2}}}{\sigma_1\sigma_2\sigma_3\pi},$$

so that

$$P(0,z) \sim u_0 - [2(1-z)]^{\frac{1}{2}}/\sigma_1\sigma_2\sigma_3\pi + O(1-z). \quad \text{(D.6)}$$

It is much harder to calculate the term of $O(1-z)$. It has only been done for the simple cubic lattice. Since

$$1/\sigma_1\sigma_2\sigma_3 = \begin{cases} 3^{\frac{1}{2}} & \text{sc},\\ 1 & \text{bcc},\\ (\frac{3}{2})^{\frac{1}{2}} & \text{fcc}. \end{cases} \quad \text{(D.7)}$$

we find that for bcc

$$P(0,z) \sim \frac{1}{4\pi^3}\{\Gamma(\tfrac{1}{4})\}^4 - \frac{1}{\pi}[\tfrac{1}{2}(1-z)]^{\frac{1}{2}} + \cdots; \quad \text{(D.8a)}$$

for fcc

$$P(0,z) \sim \frac{9\{\Gamma(\frac{1}{3})\}^6}{2^{11/3}\pi^4} - \frac{3^{\frac{1}{2}}}{4\pi}(1-z)^{\frac{1}{2}} + \cdots. \quad \text{(D.8b)}$$

More terms have been obtained for the sc lattice[11]:

$$P(0,z) \sim 1.516386 - \frac{3}{\pi}\left(\frac{3}{2}\right)^{\frac{1}{2}}(1-z)^{\frac{1}{2}} + 1.384761(1-z) - \frac{9}{4\pi}\left(\frac{3}{2}\right)^{\frac{1}{2}}(1-z)^{\frac{3}{2}} + \cdots. \quad \text{(D.9)}$$

Analytic Continuation of $a(\ell, s)$ for Re $\ell < N$*

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The positions of the singularities of the partial wave amplitude in the complex ℓ plane are investigated for that case of a relativistic, two-particle elastic scattering amplitude satisfying the Mandelstam representation. For a finite number of intermediate states it is shown that the convex hull of singularities in the ℓ plane is related to a growth indicator function. For an infinite number of intermediate states it is demonstrated that the imaginary parts of the singularities in the ℓ plane are unbounded from either above or below.

I. INTRODUCTION

THE concept of complex angular momentum was first introduced by Regge in connection with nonrelativistic potential scattering.[1] It has recently been applied to relativistic elementary particle scattering where the momentum transfer of one channel is the total energy in the crossed channel.[2] Its usefulness for several different purposes has been well established in nonrelativistic potential scattering.

One can show in potential scattering that bound states and resonances are associated with poles in the angular-momentum plane. This fact leads to the conjecture that all elementary particles and resonances are associated with moving poles in the complex angular-momentum plane.[3] Furthermore, the asymptotic behavior (large energy) of the cross section is related to the singularities in the complex angular-momentum plane.[4]

The purpose of this paper is to investigate the positions of the singularities of the partial wave amplitude in the left half of the complex-ℓ (i.e., angular-momentum) plane from the point of view of axiomatic S-matrix theory.

Before proceeding, we briefly summarize some essential properties of the partial wave amplitude in the complex angular momentum plane.

Regge has shown that the partial wave amplitude for a superposition of Yukawa potentials is a meromorphic function of ℓ in the half-plane Re $\ell \geq -\frac{1}{2}$. If r times the potential has a certain number of finite derivatives at $r = 0$, then the partial wave amplitude can be analytically continued to Re $\ell < -\frac{1}{2}$, the distance depending linearly on the number of finite derivatives of r times the potential.[5] In the region Re $\ell > -\frac{1}{2}$, when the nonrelativistic energy $E > 0$, the poles lie in the upper half-plane, and for $E < 0$ the poles lie on the real axis. When we are able to continue analytically the partial wave amplitude to Re $\ell < -\frac{1}{2}$, the poles need not lie on the real axis when $E < 0$. If they do not, however, they must occur in complex conjugate pairs.[6] When $E > 0$ and Re $\ell < -\frac{1}{2}$, the poles need not generally lie in the upper half-plane.[5]

In axiomatic S-matrix theory, if the validity of the Mandelstam representation is assumed, then a suitable continuation in the complex ℓ plane can be defined for Re $\ell \geq N$ where N is the number of subtractions needed in the Mandelstam representation.[7] The partial wave amplitude is holomorphic for Re $\ell > N$. The existence and properties of Regge poles for Re $\ell < N$ have so far not been established rigorously except for some tentative results in the elastic unitarity approximation[8] and for special cases where the crossed channel is neglected.[9]

In this paper we restrict ourselves to the case of elastic pion–pion scattering without consideration of isospin, and assume that the elastic scattering amplitude obeys the Mandelstam representation. These restrictions are introduced for the sake of simplicity and are not crucial to the proof. The

* This work was conducted under the auspices of the U. S. Atomic Energy Commission.
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[1] T. Regge, Nuovo Cimento **14**, 951 (1959).
[2] See, for example, G. F. Chew and S. C. Frautschi, Phys. Rev. Letters **7**, 394 (1961).
[3] R. Blankenbecker and M. L. Goldberger, Phys. Rev. **126**, 1202 (1962), and G. F. Chew and S. C. Frautschi, Phys. Rev. Letters **8**, 41 (1962).
[4] See, for example, V. N. Gribov, Nucl. Phys. **40**, 107 (1963).
[5] R. G. Newton, J. Math. Phys. **3**, 867 (1962); **4**, 1342 (1963).
[6] B. R. Desai and R. G. Newton, Phys. Rev. **129**, 1445 (1963).
[7] See, for example, A. Martin, Phys. Letters **1**, 72 (1962).
[8] See, for example, R. Oehme, Phys. Rev. Letters **9**, 358 (1962).
[9] A. O. Barut, "Analyticity in Angular Momentum of the Relativistic Many Channel S Matrix from Dispersion Relations and Unitarity," University of California preprint.

latter is based only on the analytic properties of the elastic scattering amplitude.

In Sec. II we outline what is meant by the Mandelstam representation. We define the partial wave amplitude $a_\ell(s)$ and relate its singularities in the complex ℓ plane to the Mellin transform of the absorptive part of the elastic scattering amplitude. In Sec. III we relate the Mellin transform of the absorptive part of the elastic scattering amplitude to its Laplace transform. To make the procedure clear, we first consider a case where the elastic scattering amplitude for fixed s has only a finite number of branch points in the complex t plane. We then rotate the path of integration of the Laplace transform of the absorptive part of the elastic scattering amplitude in the complex t plane and, hence, analytically continue the partial wave amplitude to a larger region. In Sec. IV we consider the general case for which the elastic scattering amplitude has an infinite number of intermediate states (i.e., branch points). Since the branch points run to + and − infinity along the real axis of the t plane we will not be able to rotate the path of integration of the Laplace transform of the absorptive part of the elastic scattering amplitude as we did for the case of a finite number of branch points. From this property we are able to show that the imaginary part of the singularities in the ℓ plane are neither bounded above nor below.

II. PARTIAL WAVE AMPLITUDE

Consider the reactions shown in Fig. 1 and given below

$$\begin{aligned} &1:\ \pi(P_1) + \pi(P_2) \to \pi(P_3) + \pi(P_4), \\ &2:\ \pi(P_1) + \pi(-P_4) \to \pi(P_3) + \pi(-P_2), \\ &3:\ \pi(P_1) + \pi(-P_3) \to \pi(-P_2) + \pi(P_4), \end{aligned} \tag{1}$$

and define in the usual manner

$$\begin{aligned} &(\hbar = c = m_\pi = 1), \qquad s = -(P_1 + P_2)^2, \\ &t = -(P_1 - P_4)^2, \qquad u = -(P_1 - P_3)^2, \end{aligned} \tag{2}$$

where $s + t + u = 4$ and P_i is the 4-momentum of the ith particle.

Let $A(s, t, u)$ be a function of three complex variables of which two are independent. Define it to be holomorphic except in the following regions:

(1) $s > 4$ and real for all t; when $s = 4$, the $A(s, t, u)$ has a branch point with the cut running from 4 to ∞. Likewise at $s = (2n)^2$ for $n = 1, 2, 3, \cdots, \infty$ there are branch points with cuts running from $(2n)^2$ to ∞.

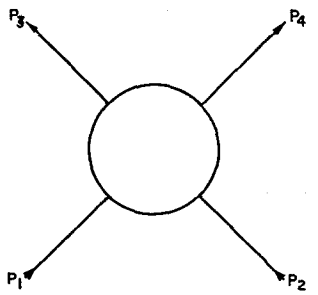

FIG. 1. Diagram describing the pion–pion elastic scattering amplitude.

(2) $t > 4$ and real for all u; when $t = 4$, then $A(s, t, u)$ has a branch point with the cut running from 4 to ∞. Likewise at $t = (2n)^2$ for $n = 1, 2, 3, \cdots, \infty$ there are branch points with cuts running from $(2n)^2$ to ∞.

(3) $u > 4$ and real for all s; when $u = 4$, then $A(s, t, u)$ has a branch point with the cut running from 4 to ∞. Likewise at $u = (2n)^2$ for $n = 1, 2, 3, \cdots, \infty$ there are branch points with cuts running from $(2n)^2$ to ∞.

The elastic scattering amplitude for the three processes of Fig. 1 is described by the one function $A(s, t, u)$ in the following way[10]:

$$\begin{aligned} &A_{\mathrm{I}}(s, t) = \lim_{\epsilon \to 0} A(s + i\epsilon, t, u) \\ &\qquad \text{where } t < 0 \text{ and real; } s > 4 \text{ and real,} \\ &A_{\mathrm{II}}(t, u) = \lim_{\epsilon \to 0} A(s, t + i\epsilon, u) \\ &\qquad \text{where } t > 4 \text{ and real; } u < 0 \text{ and real,} \\ &A_{\mathrm{III}}(u, s) = \lim_{\epsilon \to 0} A(s, t, u + i\epsilon) \\ &\qquad \text{where } u > 4 \text{ and real; } s < 0 \text{ and real.} \end{aligned} \tag{3}$$

Let us consider the amplitude $A(s, t, u)$ as a function of t for an arbitrary fixed s. The singularities of $A(s, t, u)$ in the complex t plane are shown in Fig. 2.

To construct the analytic function $A(s, t, u)$ in terms of a Mandelstam representation, with a finite number of subtraction constants, it is necessary for fixed s that $\lim_{t \to \infty} |A(s, t, u)| \leq t^m$. The power of m can be arbitrarily large, but must be finite.[11] For the proof that follows, we must strengthen this condition and assume that $|A(s, t, u)|$ is not only bounded by a large but finite power of $|t|$ but also that this power m' is not an integer. [The reason we must

[10] J. C. Taylor, "Special Topics in Dispersion Relations," NYO-9364, New York University.

[11] M. Surgawara and A. Kanazawo, Phys. Rev. **123**, 1895 (1961).

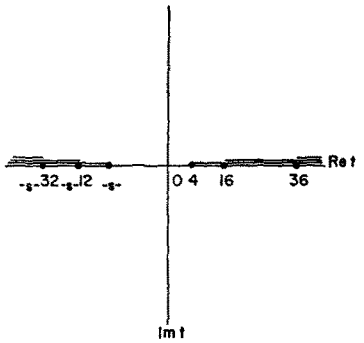

FIG. 2. Singularities of $A(s, t)$ for fixed s in the complex t plane.

strengthen this condition will become evident in Eq. (24). We want to take the Mellin transform of a function $B^m(s, t)$ which is closely related to $A(s, t, u)$. In order for this to be defined, the following two conditions must be satisfied:

$$|A(s, t, u)| \underset{\substack{t\to\infty \\ s \text{ fixed}}}{\to} O(|t|^{X_1}),$$

$$|A(s, t, u)| \underset{\substack{t\to 0 \\ s \text{ fixed}}}{\to} O(|t|^{X_2}),$$

where $X_2 < X_1$. Since $A(s, t, u)$ is analytic at $t = 0$, this implies that X_2 must be a positive integer. We also have that $X_1 < X_2 + 1$ from Eq. (23), so that X_1 cannot be an integer.] This is not a very restrictive condition since if $|A(s, t, u)|$ does go asymptotically as $|t|^{m'}$ for some fixed s, we only need to change s until the above assumption is satisfied.

We first consider a case where $A(s, t, u)$ has an arbitrary but finite number m of branch points on either cut (see Fig. 2). For convenience we assume that both cuts have the same number of branch points. The function so defined is called $A^m(s, t, u)$.

Applying the Cauchy integral theorem to $A^m(s, t, u)$ with the smallest number N of subtractions needed for convergence, we obtain for fixed s,

$$A^m(s, t, u) = \frac{t^N}{\pi}\int_4^\infty \frac{A_t^m(s, t')\,dt'}{(t' - t)t'^N} + \frac{u^N}{\pi}\int_4^\infty \frac{A_u^m(s, u')\,du'}{(u' - u)u'^N} + \mathcal{P}_{N-1}^m(t). \quad (4)$$

$A_u^m(s, u)$ and $A_t^m(s, t)$ are the discontinuities across the left-hand and right-hand cuts, respectively; i.e.,

$$A_u^m(s, u) = \lim_{\epsilon\to 0}[A^m(s, u + i\epsilon) - A^m(s, u - i\epsilon)]/2i \quad (5a)$$

for $t < -s$, and

$$A_t^m(s, t) = \lim_{\epsilon\to 0}[A^m(s, t + i\epsilon) - A^m(s, t - i\epsilon)]/2i \quad (5b)$$

for $t > 4$. $\mathcal{P}_{N-1}^m(t)$ is a polynomial of degree $N - 1$ in the variable t.

For a finite number of branch points we will assume that crossing symmetry is still true[12]; i.e.,

$$A_t^m(s, t) = A_u^m(s, t). \quad (6)$$

We have thus succeeded in constructing an analytic function $A^m(s, t, u)$ which is holomorphic in the cut t plane[13] for fixed s and has m branch points. To include all the branch points we must take the limit of the sequence $\{A^m(s, t, u)\}$ for $m \to \infty$. It follows that

$$A(s, t, u) = \lim_{m\to\infty}\{A^m(s, t, u)\}. \quad (7)$$

$A(s, t, u)$ has the required properties of the Mandelstam representation, as stated below Eq. (2), and has the integral representation

$$A(s, t, u) = \frac{t^N}{\pi}\int_4^\infty \frac{A_t(s, t')\,dt'}{(t' - t)t'^N} + \frac{u^N}{\pi}\int_4^\infty \frac{A_u(s, u')\,du'}{u'^N(u' - u)} + \mathcal{P}_{N-1}(t), \quad (8)$$

where

$$A_t(s, t) = \lim_{m\to\infty} A_t^m(s, t),$$
$$A_u(s, u) = \lim_{m\to\infty} A_u^m(s, u), \quad (9)$$
$$\mathcal{P}_{N-1}(t) = \lim_{m\to\infty} \mathcal{P}_{N-1}^m(t),$$

and N is the minimum number of subtractions needed for convergence of Eq. (8).

The partial wave amplitude can be defined by

$$a_l(s) = \frac{1}{2}\int_{-1}^{+1} dZ P_l(Z) A(s, t, u), \quad (10)$$

where $Z = 1 + 2t/(s - 4)$ for fixed $s \geq 4$. From Eq. (8) it follows that $a_l(s)$ is

$$a_l(s) = \frac{1}{2}\int_{-1}^{+1} dZ P_l(Z)\left\{\sum_{n=0}^{N-1} b_n(s)\mathcal{P}_n\left[\frac{(Z-1)(s-4)}{2}\right] + \frac{[\frac{1}{2}(Z-1)(s-4)]^N}{\pi} \times \int_4^\infty \frac{dt' A_t(s, t')}{t'^N[t' - \frac{1}{2}(Z-1)(s-4)]} + \frac{[-\frac{1}{2}(Z+1)(s-4)]^N}{\pi} \times \int_4^\infty \frac{du' A_u(s, u')}{u'^N[u' + \frac{1}{2}(Z+1)(s-4)]}\right\}, \quad (11)$$

[12] F. M. Kuni and I. D. Terentiv, Soviet Phys.—JETP **13**, 607 (1961) [Zh. Eksperim. i Teor. Fiz. **40**, 866 (1961)].

[13] The cut t plane is defined to be all those values of complex t outside the portion real axis $t \geq 4$ and $t \leq -s$; i.e., $\{t: t \notin [4, \infty) \text{ and } [-s, -\infty)\}$.

where b_n is the nth coefficient of the polynomial $\mathcal{P}_{N-1}(t)$.

For Re $\ell \geq N$ the order of integration in Eq. (11) can be interchanged, and we get the Froissart-Gribov formula[14]

$$\alpha_\ell(s) = \frac{[1 + (-1)^\ell]2}{\pi(s-4)} \times \int_4^\infty dt\, Q_\ell\left(1 + \frac{2t}{s-4}\right) A_t(s, t), \qquad (12)$$

where $Q_\ell(Z)$ is a Legendre polynomial of the second kind and has the following properties[15]:

$$Z^m Q_\ell(Z) = \frac{1}{2}\int_{-1}^{+1} dx \frac{P_\ell(x)x^m}{Z - x} \quad \text{for} \quad \ell \geq m, \qquad (13a)$$

$$Q_\ell(Z) = \frac{2^\ell[\Gamma(\ell+1)]^2}{\Gamma(2\ell+2)}\left(\frac{2t}{s-4}\right)^{-\ell-1} \times {}_2F_1\left(1+\ell, 1+\ell; 2+2\ell; -\frac{s-4}{t}\right) \qquad (13b)$$

and

$${}_2F_1\left(1+\ell, 1+\ell; 2\ell+2; -\frac{s-4}{t}\right) = \sum_{n=0}^{\infty} \frac{\Gamma^2(1+l+n)\Gamma(2\ell+2)[-(s-4)/t^n]}{\Gamma^2(\ell+1)\Gamma(2\ell+2+n)n!} \qquad (13c)$$

for $|(s-4)/t| < 1$.

To study the analytic properties of $\alpha_\ell(s)$ it is useful to recast Eq. (12) in the form

$$\alpha_\ell(s) = \frac{[1+(-1)^\ell](s-4)^\ell\Gamma^2(\ell+1)}{\pi\Gamma(2\ell+2)} \times \left\{\int_4^\infty dt\, t^{-\ell-1}A_t(s,t) \times {}_2F_1\left(\ell+1, \ell+1; 2\ell+2; -\frac{s-4}{t}\right)\right\}. \qquad (14)$$

In principle, $\alpha_\ell(s)$ should now be separated for even and odd ℓ for the sake of analytically continuing the two amplitudes separately.[16] However, for odd integer ℓ, it is clear that $\alpha_\ell(s) = 0$, so we only need to consider the case of even ℓ. In this case, Eq. (14) reduces to

$$\alpha_\ell(s) = 2(s-4)^\ell\Gamma^2(\ell+1)/\pi\Gamma(2\ell+2) \times \left\{\int_4^\infty dt\, t^{-\ell-1}A_t(s,t) \times {}_2F_1\left(\ell+1, \ell+1; 2\ell+2; -\frac{s-4}{t}\right)\right\}. \qquad (15)$$

[14] V. N. Gribov, Soviet Phys.—JETP **15**, 871 (1962) [Zh. Eksperim. i Teor. Fiz. **41**, 1221 (1962)].

[15] Bateman Manuscript Project, California Institute of Technology, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1.

[16] See, for example, A. Martin, Phys. Letters **1**, 72 (1962).

Equation (15) can be used to define an analytic function $\alpha(\ell, s)$ in the complex ℓ plane for Re $\ell \geq N$, which coincides with the partial wave amplitude $\alpha_\ell(s)$ for even integer values of ℓ. Furthermore, it has been shown that $\alpha(\ell, s)$ is holomorphic for Re $\ell \geq N$.[16] We also assume that Eq. (15) defines a correct analytic continuation of $\alpha(\ell, s)$. That is to say, the analytic continuation defined by Eq. (15) for Re $\ell \geq N$, agrees with the given $\alpha_\ell(s)$ of Eq. (10) when Eq. (15) is continued to integers less than N.

In order to study the analytic properties of $\alpha(\ell, s)$ for Re $\ell < N$, we would like to have a simpler expression than Eq. (15). To construct one which contains only the leading singularities (i.e., the singularities farthest to the right) in the ℓ plane, we separate from ${}_2F_1[1+\ell, 1+\ell; 2\ell+2; -(s-4)/t]$ the first few terms of its asymptotic expression as $t \to \infty$. These terms are denoted by g_n below.

Let

$$\begin{aligned} &{}_2F_1(\ell+1, \ell+1; 2\ell+2; -(s-4)/t) \\ &= \left\{{}_2F_1[\ell+1, \ell+1; 2\ell+2; -(s-4)/t] - \sum_{k=0}^{h} \frac{\Gamma^2(\ell+1+k)\Gamma(2\ell+2)[-(s-4)/t]^k}{\Gamma(2\ell+2+k)k!\,\Gamma^2(\ell+1)}\right\} \\ &\quad + \sum_{k=0}^{h} \frac{\Gamma^2(\ell+1+k)\Gamma(2\ell+2)[-(s-4)/t]^k}{\Gamma(2\ell+2+k)k!\,\Gamma^2(\ell+1)} \\ &= g_0(s, t, \ell) + g_h(s, t, \ell), \end{aligned} \qquad (16)$$

where

$$g_0(s, t, \ell) = {}_2F_1[\ell+1, \ell+1; 2\ell+2; (4-s)/t] - \sum_{k=0}^{h} \frac{\Gamma^2(\ell+k+1)\Gamma(2\ell+2)[(4-s)/t]^k}{\Gamma^2(\ell+1)k!\,\Gamma(2\ell+2+k)}$$

and

$$g_h(s, t, \ell) = {}_2F_1[\ell+1, \ell+1; 2\ell+2; (4-s)/t] - g_0(s, t, \ell).$$

Equation (15) then becomes

$$\alpha_\ell(s) = \frac{2(s-4)^\ell\Gamma^2(\ell+1)}{\pi\Gamma(2+2)} \times \left\{\int_4^\infty dt g_0(s, t, \ell)A_t(s, t)t^{-\ell-1} + \int_4^\infty dt g_h(s, t, \ell)A_t(s, t)t^{-\ell-1}\right\} \qquad (17)$$

for Re $\ell \geq N$.

The first term in the braces of Eq. (17) is holomorphic in ℓ for Re $\ell > N - h - 1$. [Since

$$g_0(s, t, \ell) \underset{t\to\infty}{\to} O(t)^{-h-1} \quad \text{and} \quad |A(s, t)| \underset{t\to\infty}{\leq} O(t)^N,$$

it follows that

$$\left|\int_4^\infty dt\, g_0(s, t, \ell)A(s, t)t^{-\ell-1}\right| \leq \int_4^\infty dt\, |g_0(s, t\ell)|\, |A(s, t)|\, t^{-\ell-1} < \infty$$

for Re $\ell > N - h - 1$. Furthermore, since the integral is analytic in ℓ, the first term in the braces of Eq. (17) is holomorphic for Re $\ell > N - h - 1$.] Therefore, the second term in the braces of Eq. (17) contains the singularities of $\mathfrak{A}(\ell, s)$ farthest to the right in the complex ℓ plane; therefore, this is the only term we need to consider in order to continue $\mathfrak{A}(\ell, s)$ analytically to the region Re $\ell < N$.

$$\int_4^\infty dt\, g_h(s, t, \ell)A_t(s, t)t^{-\ell-1} = \sum_{k=0}^{h} \frac{\Gamma^2(\ell+1+k)\Gamma(2\ell+1)(4-s)^k}{\Gamma^2(\ell+1)k!\,\Gamma(2\ell+2+k)} \times \int_4^\infty t^{-\ell-1-k}A_t(s, t)\, dt. \tag{18}$$

Equation (18) shows that the analyticity of $\mathfrak{A}(\ell, s)$ in the complex ℓ plane is related to the Mellin transform of the absorptive part of the amplitude.[17]

III. ANALYTIC CONTINUATION FOR A FINITE NUMBER OF INTERMEDIATE STATES

In this section we will, for heuristic reasons, replace $A_t(s, t)$ by $A_t^m(s, t)$ as defined in Sec. I and study the resulting analytic properties of $\mathfrak{A}(\ell, s)$. This is equivalent to considering the elastic scattering amplitude with only the first m branch points on either branch cut.

In the previous section we have shown that in order to continue $\mathfrak{A}(\ell, s)$ analytically to Re $\ell \leq N$, we need only consider the properties of the Mellin transform of the absorptive part of the elastic scattering amplitude.

We first study the holomorphic domain of the following related function[18]

$$\mathfrak{M}_{4,t}^{-\ell}[A_t^m(s, t)] \equiv \int_4^\infty A_t^m(s, t)t^{-\ell-1}\, dt. \tag{19}$$

This function, as we already know, is holomorphic for Re $\ell \geq N$. However, we still do not know if we can extend this region further. The Mellin transform of a function may have a natural boundary as shown by the following example.[19]

Let

$$F(x) = \begin{cases} k & \text{for } e^{-(k+1)^2} \leq x \leq e^{-k^2} \\ & k = 0, 1, 2, \cdots, \infty \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

So for Re $\rho > 0$

$$\mathfrak{M}_{0,x}^{\rho}[F(x)] = \int_0^\infty F(x)x^{\rho-1}\, dx = \int_0^\infty F(e^{-v})e^{-\rho v}\, dy,$$

where we have substituted $x = e^{-v}$. $F(e^{-v})$ now becomes

$$F(e^{-v}) = \begin{cases} k & \text{for } k^2 \leq y \leq (k+1)^2 \\ & k = 0, 1, \cdots, \infty \\ 0 & \text{otherwise} \end{cases} \tag{21}$$

and we find

$$\mathfrak{M}_{0,x}^{\rho}[F(x)] = \sum_{k=0}^{\infty} \int_{k^2}^{(k+1)^2} e^{-\rho v}k\, dy = \frac{1}{\rho}\sum_{k=1}^{\infty} k(e^{-k^2\rho} - e^{-(k+1)^2\rho}) = \frac{1}{\rho}\sum_{k=1}^{\infty} e^{-k^2\rho}. \tag{22}$$

This power series is known to have a natural boundary at Re $\rho = 0$.

In Eq. (19), $A_t^m(s, t)$ is only defined along the real axis. In order to study the analytic properties of the Mellin transform $\mathfrak{M}_{4,t}^{\mu}[A_t^m(s, t)]$ of $A_t^m(s, t)$, it is more convenient to define an analytic function $B^m(s, t)$ of t, the Mellin transform of which is related to $\mathfrak{M}_{4,t}^{\mu}[A_t(s, t)]$. For computing $\mathfrak{M}_{0,t}^{\mu}[B^m(s, t)]$, the path of integration may be varied, which we cannot do for $\mathfrak{M}_{4,t}^{\mu}[A_t^m(s, t)]$. $B^m(s, t)$ is

$$B^m(s, t) = \frac{t^N}{\pi}\int_4^\infty \frac{A_t^m(s, t')\, dt'}{t'^N(t' - t)} + \frac{(-t)^N}{\pi}\int_4^\infty \frac{A_t^m(s, t')\, dt'}{t'^N(t' + t)}, \tag{23}$$

where $A_t^m(s, t)$ is defined in Sec. I. The function $B^m(s, t)$ has the following properties:

(1) $|B^m(s, t)| \to O(|t|^{N'})$ as $|t| \to \infty$. This follows from the fact that $|B^m(s, t)| = O(|A^m(s, t, u)|)$ as $|t| \to \infty$, and we have assumed that $|A^m(s, t, u)| \to O(|t|^{N'})$ where $N - 1 < N' < N$, since N is the

[17] This relation between the singularities of the partial wave amplitude and the Mellin transform of the absorptive part of the elastic scattering amplitude was also pointed out by A. O. Barut and D. E. Zwanziger in Phys. Rev. **127**, 974 (1962). M. Froissart also used the Mellin transform in studying the complex angular momentum in potential scattering in J. Math. Phys. **3**, 922 (1962).

[18] Since k is an integer in Eq. (18), we can absorb it in l.

[19] G. Doetsch, *Handbuch der Laplace Transformation* (Verlag Berkhauser, Basel, 1950), Vol. I, p. 151.

minimum number of subtractions needed for convergence in Eq. (4).

(2) $B^m(s, t)$ is a holomorphic function in the t plane except for a right-hand cut running to ∞ and branch points at $(2n)^2$ where $n = 1, 2, \cdots, m$ and a left-hand cut running to $-\infty$ with branch points at $(-2n)^2$ where $n = 1, 2, \cdots, m$.

Consider the Mellin transform of $B^m(s, t)$ where the path of integration is from zero to infinity at an angle θ to the real axis where $0 < \theta < \pi$. We obtain (see Appendix A)

$$\mathfrak{M}^{\mu}_{0,t}[B^m(s, t)] = \frac{[(-1)^N + (-1)^{\mu-1}]}{\sin(\pi\mu)} \{\mathfrak{M}^{\mu}_{4,t}[A^m_t(s, t)]\}, \quad (24)$$

where, for convenience, we have introduced $\mu = -\ell$.[20] Since $\mathfrak{M}^{\mu}_{4,t}[A^m_t(s, t)]$ is analytic for $\mu < -N'$ and $1/\sin(\pi\mu)$ is analytic everywhere except when μ is an integer or zero, then $\mathfrak{M}^{\mu}_{0,t}[B^m(s, t)]$ is analytic for $-N < \mu < -N'$ (see Fig. 3) with N' not an integer.

With the use of Eq. (24) we obtain the more convenient representation of $\mathfrak{M}^{\mu}_{t,4}[A^m_t(s, t)]$ discussed before:

$$\mathfrak{M}^{\mu}_{4,t}[A^m_t(s, t)] = \frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \mathfrak{M}^{\mu}_{0,t}[B^m(s, t)]$$

$$= \frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_0^{(2m)^2 e^{i\theta}} B^m(s, t) t^{\mu-1}\, dt$$

$$+ \frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_{(2m)^2 e^{i\theta}}^{\infty} B^m(s, t) t^{\mu-1}\, dt, \quad (25)$$

where $0 < \theta < \pi$.

The reason that this representation is more convenient is that $C^m(s, t)$ is defined everywhere in the upper half of the complex t plane, whereas $A^m_t(s, t)$ is only defined for real t.

We demonstrate that the first term on the right-hand side of Eq. (25) is an entire function of μ. Consider the region Re $\mu > -N$. Then

$$\frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_0^{(2m)^2 e^{i\theta}} t^{\mu-1} B^m(s, t)\, dt \quad (26)$$

has an integrand which is holomorphic in μ. Since $|B^m(s, t)| \to O(|t|^N)$ as $t \to 0$ [see Eq. (23)], the integrand is continuous for all t on the path of integration if $\mu < -N$. Furthermore, the path of integration is rectifiable, so that the integral in Eq. (26) defines a function of μ which is analytic for Re $\mu > -N$. A path is rectifiable if it is of finite length; e.g., $|\int_0^{(2m)^2 e^{i\theta}} dt| = (2m)^2 < \infty$.

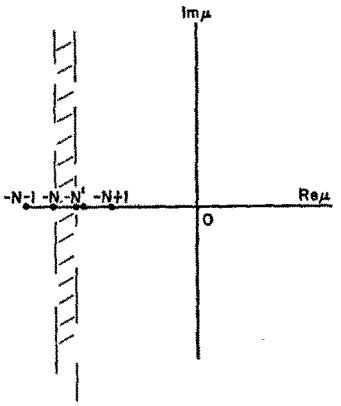

FIG. 3. Region of analyticity of the Mellin transform of $C^m(s, t)$ in the complex μ plane.

Now consider a case where Re $\mu < N'$. From Eq. (25) we find

$$\frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_0^{(2m)^2 e^{i\theta}} t^{\mu-1} B^m(s, t)\, dt$$

$$= \frac{-\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_{(2m)^2 e^{i\theta}}^{\infty} t^{\mu-1} B^m(s, t)\, dt$$

$$+ \int_4^{\infty} A^m_t(s, t) t^{\mu-1}\, dt. \quad (27)$$

Since

$$|B^m(s, t)| \to O(|t|^{N'}) \quad \text{as} \quad |t| \to \infty,$$

$$|A^m_t(s, t)| \to O(|t|^{N'}) \quad \text{as} \quad |t| \to \infty$$

and

$$|B^m(s, t)| \to O(1) \quad \text{as} \quad t \to (2m)^2 e^{i\theta},$$

$$|A^m_t(s, t)| \to O(1) \quad \text{as} \quad t \to 4,$$

both integrals on the right-hand side of Eq. (27) converge for Re $\mu < -N'$ and Eq. (27) defines a holomorphic function in this region. Hence

$$\frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_0^{(2m)^2 e^{i\theta}} t^{\mu-1} B^m(s, t)\, dt \quad (28)$$

is an entire function in the μ plane. Using this fact we only need to consider the second term in Eq. (25) which is

$$\frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_{(2m)^2 e^{i\theta}}^{\infty e^{i\theta}} dt B^m(s, t) t^{\mu-1}.$$

With the transformation $t = e^w (2m)^2 e^{i\theta}$, we find

$$\int_{(2m)^2 e^{i\theta}}^{\infty} B^m(s, t) t^{\mu-1}\, dt = (2m)^2 e^{i\theta} \int_0^{\infty} dw C^m(s, w) e^{\mu w}, \quad (29)$$

[20] When we are working with the Mellin transform, we use μ as the variable, but when we are working with the Laplace transform it is more convenient to use t.

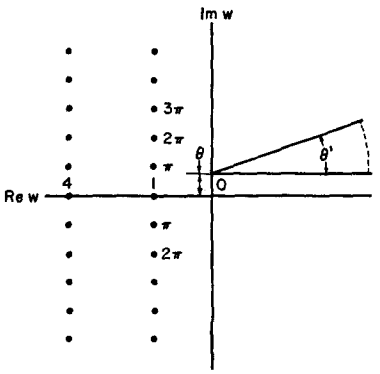

FIG. 4. Path of integration of the generalized Laplace transform of $C^m(s, w)$ in the w plane.

where $C^m(s, w) = B^m[s, e^w(2m)^2 e^{i\theta}]$ and is analytic for all Re $w \geq 0$. Reintroducing ℓ as the variable, the integral in Eq. (29) is proportional to

$$\mathfrak{L}[C^m(s, w)] \equiv \int_0^\infty C^m(s, w)e^{-w\ell}\, dw, \qquad (30)$$

where we have let $\mu = -\ell$.

Since $C^m(s, w)$ is holomorphic for Re $w \geq 0$, we can generalize the Laplace transform in Eq. (30) so that the path of integration makes an angle θ' where $-\pi/2 < \theta' < \pi/2$ with respect to the real axis in the w plane (see Fig. 4). We use the following notation:

$$\mathfrak{L}^{\theta'}[C^m(s, w)] = \int_0^{\infty e^{i\theta}} C^m(s, w)e^{-w\ell}\, dw. \qquad (30a)$$

By rotating the path of integration in the Laplace transform we see that, under certain conditions, the convergent half-plane of ℓ likewise rotates and therefore analytically continues Eq. (25) to a larger region then defined by its integral. We can therefore define $\mathfrak{A}_\ell(s)$ in a larger region.

In order to demonstrate this continuation, we make use of the following theorem:

Theorem I[21]: If $F(z)$ is analytic in a Riemann surface between the angles $\alpha < \arg z < \beta$ with the exception of $z = 0$ and $z = \infty$, and satisfies the conditions

(i) $|F(z)| \underset{r\to\infty}{<} Ae^{\alpha r}$ with $\alpha > 0$ and $z = re^{i\theta}$

(ii) $|F(z)| \underset{r\to 0}{<} Br^{-b}$ with $b < 1$,

then

$$\mathfrak{L}^\theta[F(z)] = \int_0^{\infty e^{i\theta}} e^{-\rho z}F(z)\, dz \qquad (31)$$

converges for $\alpha < \theta < \beta$ and Re $(\rho e^{i\theta}) > \alpha$. These are the collection of half-planes which are perpendicular to the ray of length α along θ and bounded by $\alpha < \theta < \beta$ (see Fig. 5). All of these integrals, $\mathfrak{L}^\theta[F(z)]$, are elements of the same analytic function and therefore form the basis of analytic continuation.

There exist many different possibilities for the convex hull of singularities of $\mathfrak{L}^\theta[C^m(s, w)]$. To show this we even limit ourselves to the special case that $C^m(s, w)$ is of the exponential type for Re $w \geq 0$; that is, we assume that there exists a constant b such that

$$|C^m(s, w)| \leq e^{b|w|} \quad \text{for} \quad \text{Re } w \geq 0. \qquad (32)$$

Using Theorem I, we note that in this special case $\mathfrak{L}^\theta[C^m(s, w)]$ is holomorphic, at least outside the horizontal left-half strip

$$\text{Re } \ell \leq b, \qquad |\text{Im } \ell| \leq b. \qquad (33)$$

In order to enlarge its holomorphic domain, we will define the growth indicator[22] of $C^m(s, w)$ as

$$V(\phi, s) = \lim_{|w|\to\infty} \sup_{\phi} \left(\frac{\log |C^m(s, |w|e^{i\phi})|}{|w|}\right) \qquad (34)$$

for $-\pi/2 \leq \phi \leq \pi/2$.

Consider the half-planes H_ϕ, defined by

$$\text{Re } (\ell e^{i\phi}) \leq V(\phi, s), \qquad -\pi/2 \leq \phi \leq \pi/2, \qquad (35)$$

where at the endpoints we replace $V(\phi, s)$ by its limits. The intersection of all the H_ϕ within the region of allowed ϕ, defines a region T; i.e.,

$$T = \bigcap_\phi H_\phi. \qquad (36)$$

Then by means of Theorem I it can be shown that T is the convex hull of singularities[22,23] of $\mathfrak{L}^\theta[C^m(s, w)]$;

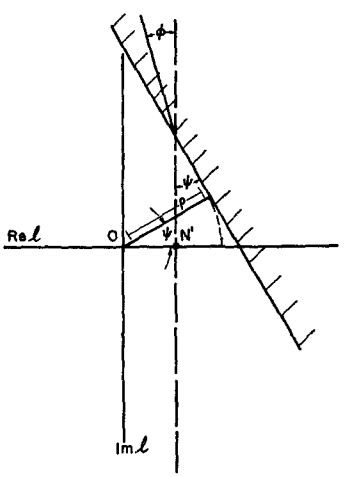

FIG. 5. Rotated boundary showing the region of analyticity of the Laplace transform of $C(s, w)$ in the ℓ plane.

[21] See Ref. 19, p. 366.

[22] See Ref. 19, p. 378.

[23] E. Hille, *Analytic Function Theory* (Ginn and Company, Boston, Massachusetts, 1962), Vol. II, p. 463.

hence, $\mathfrak{L}^{\theta}[C^m(s, w)]$ is holomorphic in the ℓ plane with the exception of the convex domain T. Equation (34) demonstrates that many possibilities exist for $V(\phi, s)$, and hence for T, since $C^m(s, w)$ can have various asymptotic forms. Consideration of Eqs. (24), (25), (28), (30), and Theorem I gives us all the convex hull of singularities of Eq. (19). Since h is arbitrary in Eqs. (17) and (18), even for a finite number m of intermediate states in the elastic scattering amplitude, the convex hull of singularities of $\mathfrak{a}_\ell(s)$ is determined by the singularities of Eq. (19). Exceptions are possible additional poles on the real axis at the negative integers.

The convex hull of singularities of $\mathfrak{a}(\ell, s)$ may be constructed from that of $\mathfrak{M}^{\mu}_{4,s}[A^m_t(s, t)]$ as follows.

Let T^h be the convex hull of singularities of $\mathfrak{M}^{-(l+h)}_{4,s}[A^m_t(s, t)]$. From Eq. (17) it follows that the convex hull of singularities of $\mathfrak{a}(\ell, s)$ for Re $\ell > N - h - 1$ is the union of all T^k for $k = 0, 1, 2, \cdots, h$; i.e.,

$$\bigcup_{k=0,1\cdots h} T^k.$$

Since h is arbitrary, we can let it be as large as we like, hence $\bigcup_k T^k$ for all k is the convex hull of singularities of $\mathfrak{a}(\ell, s)$ in this special case of finite m.

From the remarks above, we see that the position of the singularities of $\mathfrak{a}(\ell, s)$ in the ℓ plane requires knowledge of the growth indicator function of $C^m(s, w)$. For an infinite number of intermediate states in the elastic scattering amplitude, the domain of singularities of $\mathfrak{a}(\ell, s)$ in the ℓ plane is not as arbitrary as for a finite number of intermediate states. In fact, we show that the imaginary parts of the singularities are unbounded.

IV. CONTINUATION FOR AN INFINITE NUMBER OF INTERMEDIATE STATES

Let us now consider the general case where the elastic scattering amplitude has an infinite number of branch points. In this case we are not able to proceed exactly as we did before. We cannot rotate the path of integration in the Laplace transform as we did in Eq. (30a) and hence we won't be able to use Theorem I to analytically continue to a larger domain. We are unable to rotate the path of integration because regardless of the point we rotate about or how small the amount of rotation, we will always run into a singularity since singularities extend all the way to infinity, unlike the case for a finite number of intermediate states. However, from this observation we will be able to prove by contradiction that the imaginary parts of the singularities in the ℓ plane are neither bounded above nor below.

To show that the imaginary parts of the singularities are neither bounded above nor below, let us consider the analogue of Eq. (19) with an infinite number of intermediate states; namely,

$$\mathfrak{M}^{-\ell}_{4,t}[A_t(s, t)] = \int_4^{\infty} A_t(s, t) t^{-\ell-1}\, dt. \tag{37}$$

By a development analogous to that used earlier, we obtain an equation similar to Eq. (23):

$$\mathfrak{M}^{\mu}_{4,t}[A_t(s, t)] = \frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_0^{\infty e^{i\theta}} t^{\mu-1} B(s, t)\, dt. \tag{38}$$

The path of integration can be taken, just as before, at an angle θ, $(0 < \theta < \pi)$, to the real axis, since $C(s, t)$ is analytic in the upper half-plane and $t^{\mu}B(s, t)$ vanishes at infinity for Re $\mu < -N$.

By means of the same argument used to establish the analytic behavior of the expression (28), we can conclude that

$$\frac{\sin(\pi\mu)}{[(-1)^N + (-1)^{\mu-1}]} \int_0^{e^{i\theta}} t^{\mu-1} B(s, t)\, dt \tag{39}$$

is an entire function in the μ plane. Hence all the singularities will be contained in the term

$$\int_{e^{i\theta}}^{\infty e^{i\theta}} t^{\mu-1} B(s, t)\, dt. \tag{40}$$

With the substitution $t = e^{w+i\theta}$ and $\mu = -\ell$, Eq. (40) becomes

$$e^{-i\ell\theta} \int_0^{\infty} e^{-\ell w} C(s, w)\, dw = e^{-i\ell\theta} \mathfrak{L}_{\theta}[C(s, w)], \tag{41}$$

where $C(s, w) = B(s, e^{i\theta}e^{w})$ and we have defined $\mathfrak{L}_{\theta}[C(s, w)]$ as a holomorphic function in the ℓ plane for Re $\ell > N$:

$$\mathfrak{L}_{\theta}[C(s, w)] \equiv \int_0^{\infty} e^{-\ell w} C(s, w)\, dw. \tag{42}$$

It has the following properties[24]

$$|\mathfrak{L}_{\theta}[C(s, w)]| \leq \text{const}\, e^{-\theta \operatorname{Im} \ell} \quad \text{for} \quad \operatorname{Im} \ell \geq 0 \quad \text{and} \quad \operatorname{Re} \ell > N \tag{43a}$$

and

$$|\mathfrak{L}_{\theta}[C(s, w)]| \leq \text{const}\, e^{(\pi-\theta) \operatorname{Im} \ell} \quad \text{for} \quad \operatorname{Im} \ell < 0 \quad \text{and} \quad \operatorname{Re} \ell > N. \tag{43b}$$

In order to show that $\mathfrak{a}(\ell, s)$ has singularities running to infinity along the imaginary axis of the ℓ plane we assume the converse; i.e., $\mathfrak{a}(\ell, s)$ is

[24] See Ref. 19, p. 403.

holomorphic above some arbitrary point on the imaginary axis. This is equivalent to assuming that there exists an upper bound on the position of singularities of $\mathfrak{L}_\theta(s, w)$ in the ℓ plane. We show that this gives us a contradiction. Hence, there can exist no upper bound on the singularities in the ℓ plane of $\mathfrak{A}(\ell, s)$. Likewise, the same argument is true for a lower bound.

Assume that in the upper half-plane, with Re $\ell < N$, there exists an upper bound on the position of the singularities of $\mathfrak{L}_\theta[C(s, w)]$. Assuming the above, we may draw a line which touches this bound and makes an angle ψ with the vertical (see Fig. 5). Since, by assumption, $\mathfrak{L}_\theta[C(s, w)]$ contains no singularities to the right of this boundary, it will have an analytic continuation. If we call this new function $\mathfrak{L}_\theta^\psi[C(s, w)]$, then the following properties are associated with it:

(1) $\mathfrak{L}_\theta^\psi[C(s, w)]$ is an analytic continuation of $\mathfrak{L}_\theta[C(s, w)]$

(2) $\mathfrak{L}_\theta^{\psi=0}[C(s, w)] = \mathfrak{L}_\theta[C(s, w)]$.

There can exist three separate cases that we must look at. They are the following:

$$\text{(1)}\quad |\mathfrak{L}_\theta^\Psi[C(s, w)]| \leq \begin{cases} |C \exp [\eta_1 \operatorname{Im} (\ell e^{i\psi'})]|, & \operatorname{Im} \ell e^{i\psi'} \geq 0 \\ |C \exp [\eta_2 \operatorname{Im} (\ell e^{i\psi'})]|, & \operatorname{Im} \ell e^{i\psi'} < 0, \end{cases}$$

where $\eta_1 < \eta_2$ and for all ψ' such that $0 \leq \psi' < \psi$.

(2) Case 1 is not true for any ψ', $0 \leq \psi' < \psi$.

(3) Case 1 is true for some particular angle $\psi' = \phi$ where $0 < \phi < \psi$.

Case 1 can be eliminated immediately, since, if it were true, we could rotate the path of integration of $\mathfrak{L}_\theta^\Psi[C(s, w)]$ in the ℓ plane and according to Theorem I this would imply that $C(s, w)$ was analytic in the sector bounded by a line parallel to the real axis and one intersecting it at an angle $-\psi$ at $\ell = 0$. However, this can never be true since no matter how small ψ is, the triangle will always inclose a singularity of $C(s, w)$. Hence, either Case 2 or 3 must be correct if there exists an upper bound on the position of the singularities on the imaginary axis of the ℓ plane, as we assumed.

If we assume that Case 2 is true, then one of the following three conditions must be correct:

(a) $|\mathfrak{L}_\theta^\Psi[C(s, w)]| \leq \text{const } |\exp (\eta_1 \operatorname{Im} \ell e^{i\psi})|$ for $\operatorname{Im} (\ell e^{i\psi}) \geq 0$

and

$$|\mathfrak{L}_\theta^\Psi[C(s, w)]| \leq \text{const } |\exp (\eta_2 \operatorname{Im} \ell e^{i\psi})| \quad \text{for} \quad \operatorname{Im} (\ell e^{i\psi}) < 0,$$

where $\eta_1 \geq \eta_2$, $\psi > 0$ and Re $(\ell e^{i\psi}) \geq \rho > N$. Here ρ is the length of the arm perpendicular to the tilted plane (see Fig. 5).

(b) $|\mathfrak{L}_\theta^\Psi[C(s, w)]| \geq \text{const } |\exp (\eta_1 \operatorname{Im} \ell e^{i\psi})|$ for $\operatorname{Im} \ell e^{i\psi} \geq 0$

and Re $\ell e^{i\psi} \geq \rho > N$ for all $\eta_1 < \eta_2$.

(c) $|\mathfrak{L}_\theta[C(s, w)]| \geq \text{const } |\exp (\eta_2 \operatorname{Im} \ell e^{i\psi})|$ for $\operatorname{Im} \ell e^{i\psi} < 0$

and Re $\ell e^{i\psi} \geq \rho > N$ for all $\eta_1 < \eta_2$.

Assume Condition (a) to be correct and let $\psi \to 0$. This implies that

$$|\mathfrak{L}_\theta^0[C(s, w)]| = |\mathfrak{L}_\theta[C(s, w)]| \leq \text{const } e^{\eta_1 \operatorname{Im} \cdot \ell}$$

for Im $\ell \geq 0$, and that

$$|\mathfrak{L}_\theta^0[C(s, w)]| = |\mathfrak{L}_\theta[C(s, w)]| \leq \text{const } e^{\eta_2 \operatorname{Im} \ell}$$

for Im $\ell < 0$ and $\eta_1 \geq \eta_2$. However, this contradicts Eqs. (43a) and (43b).

Consider Condition (b) to be correct and again take lim $\psi \to 0$. This condition implies that

$$|\mathfrak{L}_\theta^0[C(s, w)]| = |\mathfrak{L}_\theta[C(s, w)]| \geq e^{\eta_1 \operatorname{Im} \ell}$$

for Im $\ell \geq 0$ and all $\eta_1 < \eta_2$. This contradicts Eq. (43a).

Likewise, if we assume Condition (c) to be correct and let $\psi \to 0$, this will give us a contradiction to Eq. (43b). Hence, Case 2 can never be correct.

Therefore, to complete our argument all we must show is that Case 3 can never happen.

If Case 3 is correct, we restrict our angular region to ψ' such that $0 < \psi' < \phi$ (see Fig. 5). Restricted to this smaller region, it follows from the same arguments as above that Cases 1 and 2 cannot be satisfied, since the arguments were independent of how big the sector angle was. Therefore, Case 3 must be correct in this smaller sector. We can again restrict our region to a smaller sector; i.e., $0 < \psi' < \phi'$ and continue this process until Cases 1 or 2 are correct and then we will have a contradiction, since Cases 1 and 2 can never be true, no matter how small the sector is. Hence, Case 3 must be true no matter how small a sector we choose. This gives us a contradiction, as can be seen with the use of the following theorem.

Theorem II: A function $f(z)$ which is holomorphic

in a sector of opening w and which is bounded on the boundary by $e^{\eta|z|}$ is either bounded in the closed sector by $e^{\eta|z|}$ or else

$$\limsup_{r\to\infty} \{\max |f(re^{i\psi'}) - \exp(\eta r + \beta r^{\pi/w})|\} \geq 0$$

for some $\beta > 0$.

The proof of Theorem II is found in Appendix B.

Notice also that

$$|\mathfrak{L}^{\psi}_{\theta}[C(s, w)]| \leq f(|\ell|) < \infty, \tag{44}$$

where $\ell = |\ell| e^{i(\psi'+\pi/2)}$ and independent of ψ' where $0 \leq \psi' \leq \phi$. $\phi < \psi$ is a particular angle at which Case 3 is satisfied. [One way to choose $f(|\ell|)$ would be the following: Let $f(|\ell|) = \max_{\phi} |\mathfrak{L}[C(s, w)]|$, where $\ell = |\ell| e^{i(\psi'+\pi/2)}$, $0 \leq \psi' \leq \phi$.] From the argument above, ϕ can be arbitrarily small.

Theorem II can be applied to $\mathfrak{L}^{\psi}_{\theta}[C(s, w)]$ with sector opening ϕ and $\eta = \max(\eta_1 \sin\phi, \theta)$. We notice that $\mathfrak{L}^{\psi}_{\theta}[C(s, w)]$ cannot be bounded in this closed sector by $e^{\eta|\ell|}$, since if it were, then Case 1 would be true in this sector and we know this can never happen. This implies that for every $\epsilon > 0$ there exists an r_0 such that for $r > r_0$

$$\sup \max |\mathfrak{L}^{\psi}_{\theta}[C(s, w)]| \geq \exp(\eta r + \beta r^{\pi/\phi}) - \epsilon$$

and since we can choose ϕ as small as we desire, we can always find a ϕ such that $e^{\eta r+\beta r} - \epsilon > f(r)$.$^{\psi/\phi}$ This gives us a contradiction, since

$$|\mathfrak{L}^{\psi}_{\theta}[C(s, w)]| \geq \exp(\eta r + \beta r^{\pi/\phi'}) - \epsilon > f(r)$$

which is contrary to how $f(r)$ was chosen [see Eq. (44)].

We have now succeeded in showing a contradiction of the initial assumption that there exists an upper bound on the position of the singularities of $\mathfrak{L}^{\psi}_{\theta}[C(s, w)]$ in the upper half ℓ plane for Re $\ell \leq N$. A similar argument can be used to show that there also exists no lower bound. Hence, there exists an infinite number of singularities running to infinity along the imaginary axis in both directions.

Looking at Eqs. (38) and (40), we see that Eq. (37) has the same singularities $\mathfrak{L}^{\psi}_{\theta}[C(s, w)]$. From Eq. (17) we note that the singularities of $\alpha(\ell, s)$ for Re $\ell > N - h - 1$ are the same as the singularities of $\sum_{k=0}^{h} \mathfrak{M}^{-(\ell+k)}_{4,t}[A_t(s, t)]$ except for possible additional poles on the real axis at the negative integers. Since h is arbitrary, we can let it be as large as we like. Hence, the position of the singularities of $\alpha(\ell, s)$ in the ℓ plane will be the same as those of $\sum_{k=0}^{h} \mathfrak{M}^{-(\ell+k)}_{4,t}[A_t(s, t)]$ with the possible exception mentioned previously. If there are no cancellations of singularities in the sum $\sum_{k=0}^{\infty} \mathfrak{M}^{-(\ell+k)}_{4,t}[A_t(s, t)]$, then $\alpha(\ell, s)$ will have an infinite number or singularities going from $+\infty$ to $-\infty$ along the imaginary axis just as $\mathfrak{M}^{-\ell}_{4,t}[A_t(s, t)]$.

In principle, it is possible that the singularities in the sum $\sum_{k=0}^{\infty} \mathfrak{M}^{-(\ell+k)}_{4,t}[A_t(s, t)]$ cancel. However, it is obvious that the singularities farthest to the right in the ℓ plane of $\mathfrak{M}^{-\ell}_{4,t}[A_t(s, t)]$ cannot cancel. Hence, there will still exist an infinite number of singularities running from $i\infty$ to $-i\infty$ in the ℓ plane. This concludes our proof.

V. CONCLUSION

It has been shown that if the elastic pion–pion scattering amplitude satisfies the Mandelstam representation, then for a finite number of intermediate states the convex hull of singularities of the partial wave amplitude is related to a growth indicator function. However, for an infinite number of intermediate states there are stricter conditions on the positions of the singularities of $\alpha(\ell, s)$ in the complex ℓ plane. In fact, for Re $\ell \leq N$, where N is the minimum number of subtractions needed for convergence in the Mandelstam representation, there exists an infinite number of singularities on one or more axes parallel to the imaginary one of the ℓ plane (with Re $\ell \leq N$), extending to infinity in both directions. We have not shown that this is a natural boundary nor that the singularities lie on one line; however, this may very well be the case.

This proof is not peculiar to the pion–pion elastic scattering amplitude nor of the Mandelstam representation, but is based only on the fact that the elastic scattering amplitude is an analytic function for fixed s and has branch points running to infinity along the real t axes.

ACKNOWLEDGMENTS

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APPENDIX A

To take the Mellin transform of $B^m(s, t)$ we define

$$f(t) = B^m(s, t)t^{-N}, \qquad \phi(t) = A^m_t(s, t)t^{-N}.$$

Define the Mellin transform of $f(t)$ to be

$$\mathfrak{M}(f) = \int_0^{\infty(\theta)} f(t)t^{\mu-1}\,dt, \tag{A1}$$

where the path of integration is taken along a ray from zero to infinity, making an angle θ to the real axis where $0 < \theta < \pi$.

Let $t = re^{-i\theta}$, then

$$\mathfrak{M}(f) = \int_0^\infty dr\, e^{-i\theta} r^{\mu-1} e^{-i\theta(\mu-1)} A(re^{-i\theta})$$

$$= e^{-i\theta\mu} \int_0^\infty dr\, r^{\mu-1} A(re^{-i\theta})$$

$$= \frac{e^{-i\theta\mu}}{\pi} \int_0^\infty dr\, r^{\mu-1} \int_4^\infty dt\, \phi(t) \times \left\{ \frac{1}{t - re^{-i\theta}} + \frac{(-1)^N}{t + re^{-i\theta}} \right\} \qquad \text{(A2)}$$

where we have used the equation

$$f(t) = \frac{1}{\pi} \int_4^\infty dt'\, \phi(t) \left\{ \frac{1}{t' - t} + \frac{(-1)^N}{t' - t} \right\}.$$

Interchanging the order of integration in Eq. (A2) gives

$$\mathfrak{M}(f) = \frac{e^{-i\theta\mu + i\theta}}{\pi} \int_4^\infty dt\, \phi(t) \times \int_0^\infty dr \left\{ \frac{1}{te^{i\theta} - r} + \frac{(-1)^N}{te^{i\theta} + r} \right\} r^{\mu-1}. \qquad \text{(A3)}$$

The evaluation of the second integral results in

$$\frac{1}{\pi} \int_0^\infty dr\, r^{\mu-1} \left\{ \frac{1}{te^{i\theta} - r} + \frac{1}{te^{i\theta} + r} \right\}$$

$$= \frac{1}{\sin(\pi\mu)} \{ -(-te^{i\theta})^{\mu-1} + (-1)^N (te^{i\theta})^{\mu-1} \}$$

$$= \frac{t^{\mu-1} e^{i\theta(\mu-1)}}{\sin(\pi\mu)} \{ -(-1)^{\mu-1} + (-1)^N \}. \qquad \text{(A4)}$$

Thus Eq. (A3) becomes

$$\mathfrak{M}(f) = e^{-i\theta(\mu-1)} \times \int_4^\infty \frac{dt \phi(t) t^{\mu-1} [-(-1)^{\mu-1} + (-1)^N] e^{i\theta(\mu-1)}}{\sin(\pi\mu)}$$

$$= \int_4^\infty dt\, t^{\mu-1} \frac{\phi(t)[(-1)^N - (-1)^{\mu-1}]}{\sin(\pi\mu)},$$

where $0 < \mu < N - N'$.

If $\psi(\mu)$ is the Mellin transform of f then $\psi(\mu - N)$ is the Mellin transform of $B^m(s, t)$ where $B^m(s, t)t^{-N} = f(t)$. This gives us

$$\mathfrak{M}[B^m(s, t)] = \frac{(-1)^N - (-1)^{\mu-1-N}}{\sin \pi(\mu - N)} \times \int_4^\infty dt\, t^{\mu-1-N} A_t^m(s, t).$$

If we let $\mu' = \mu - N$, then

$$\mathfrak{M}[B^m(s, t)] = \frac{(-1)^N - (-1)^{\mu'-1}}{\sin(\pi\mu')} \times \int_4^\infty dt'\, t'^{\mu'-1} A_t^m(s, t'), \qquad \text{(A5)}$$

for $0 < \mu' + N < N - N'$ or $-N < \mu' < -N'$.

APPENDIX B

Theorem II: Consider a function $f(z)$ which is holomorphic in a sector of opening w formed by the intersection of rays a and b. Ray a is defined to be the line from the origin to infinity along the positive imaginary axis. Ray b is the line from the origin to infinity making an angle $w + \pi/2$ with respect to the positive real axis, where $0 < w < \pi/2$. If $f(z)$ is bounded on the boundary by $e^{\eta(z)}$ then $f(z)$ is either bounded in the closed sector by $e^{\eta(z)}$ or else

$$\limsup_{r\to\infty} \{\max |f(re^{i\psi})| - \exp(\eta r + \beta r^{\pi/w})\} \geq 0$$

for some $\beta > 0$.

Proof: The proof of Theorem II is a trivial consequence of a theorem by Phragmen and Lindelof which says:

Theorem (Phragmen–Lindelof)[22]: A function $f(z)$ which is holomorphic in a sector of opening w and which is bounded on the boundary of the sector is either bounded in the closed sector or else

$$\limsup_{r\to\infty} \{\max |f(re^{i\theta})| - \exp(\beta r^{\pi/w})\} \geq 0$$

for some $\beta > 0$.

Define the function $g(z)$ to be $g(z) = e^{iz(\eta/\sin w)}$; then $|g(z)| \leq e^{-\eta|z|}$ on ray a and $|g(z)| \leq e^{-|z|}$. Thus, we have that $|f(z)g(z)| \leq e^{-\eta|z|} e^{+\eta|z|} \leq 1$ on ray a and $|f(z)g(z)| \leq e^{-\eta z} e \leq 1$ on ray b. Hence, we may apply the Phragmen–Lindeloh theorem to $f(z)g(z)$. Then, either $f(z)g(z)$ is bounded everywhere in the sector or else

$$\limsup_{r\to\infty} \{\max |f(re^{i\theta}) e^{i\eta z}| - \exp(\beta r^{\pi/w})\} \geq 0$$

for some $\beta > 0$.

This is obviously equivalent to

$$\limsup_{r\to\infty} \{\max |f(re^{i\theta})| - \exp(\eta r + \beta_r r^{\pi/w})\} \geq 0.$$

Effects of Finite Sample Size on the Measurement of Transport Quantities

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A determination is made of the temporal evolution of the momentum autocorrelation function for a noninteracting gas constrained by walls. A frequency-dependent dielectric constant is calculated from the latter by applying an appropriate Kubo relation. Deviations from the Drude conductivity are obtained which, for high frequency and/ or large systems, are found to be $\sim o(10^2/\beta m\omega^2 L^2)$, where L is the spatial dimension of the assembly and ω the frequency of the applied field.

A similar calculation is performed to determine the effects of boundaries upon measurements of scattering cross sections for slow neutrons. It is found that, for realistic experimental conditions, wall perturbations are unlikely to be of importance.

I. INTRODUCTION

IN theoretical investigations of the relationships between macroscopic transport phenomena and the microscopic properties of matter, it is frequently stipulated that the macroscopic system be of infinite spatial dimension. Such an assertion corresponds to assuming that boundary perturbations which might be introduced into an actual experimental measurement would be negligible, relative to contributions due to interactions between the constituent particles of the assembly of interest. Indeed, the higher the density of particles or the greater the relative strength of interactions between them, the less important should be any perturbations due to wall effects.

It is of interest to supplement these rather general qualitative remarks with explicit calculations. Ideally, one would solve the complicated finite-space n-body problems associated with transport phenomena being considered. Unfortunately, the latter is usually a very difficult task. However, by neglecting interactions between particles, thus considering only the effects of collision of particles with the walls, one can at least obtain useful upper bounds for the errors which might be introduced into measurement in virtue of the finite size of an experimental system. In the following work, we consider this question for two particular transport quantities of interest: (1) the frequency-dependent dielectric constant and (2) the cross section for the scattering of slow neutrons.

In the course of investigating the first of these phenomena, we also solve the ancillary problem of calculating the temporal evolution of the momentum autocorrelation function for a gas of noninteracting particles constrained by finite boundaries. As a model which demonstrates essential features, we choose a one-dimensional box and assume specular reflection of particles at the walls. The unconditioned probability density for locating particles in phase space is taken to be Maxwellian in momentum space and uniform in configuration space. Thus, in Sec. II, an explicit determination of the temporal behavior of the autocorrelation function for all $t \geq 0$ is obtained. It is interesting that, although no information is lost when a particle collides with a wall (as a consequence of the assumption of specular reflection, the momenta before and after collision are perfectly correlated), it is found that phase mixing introduced due to the initial distribution is sufficient to insure the temporal relaxation of the autocorrelation function. Initially positive, the latter decreases, becomes negative, and finally decays asymptotically to zero (cf. Fig. 1, below).[1]

After having obtained the momentum autocorrelation function, the dielectric constant may be calculated according to an appropriate "Kubo relation."[2,3] Thus, in Sec. III, certain aspects of the frequency dependence of the dielectric constant are investigated, emphasis being given to obtaining estimates of perturbations which might be introduced into measurement of the latter as a consequence of the finiteness of a large system.

In Sec. IV, consideration is given to a similar problem concerning the measurement of cross sections for the scattering of slow neutrons.[4,5] The

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[1] Recently, I. Oppenheim and P. Mazur (Physica, to be published) have considered the temporal evolution of the momentum autocorrelation function for Brownian motion in finite systems. Although the details of the relaxation are not explicitly calculated in the latter study, similar asymptotic behavior is discernible.
[2] M. S. Green, J. Chem. Phys. **20**, 1287 (1952); **22**, 398 (1954).
[3] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).
[4] L. Van Hove, Phys. Rev. **95**, 249 (1954).
[5] R. Glauber, Phys. Rev. **98**, 1692 (1955); *Lectures in Theoretical Physics* (Boulder Lectures), Vol. IV (Interscience Div., John Wiley & Sons, Inc., New York, 1963).

model system chosen for this calculation is the same as that described above. Scattering functions are obtained by taking space–time Fourier transforms of $G_s(\mathbf{q}, t \mid \mathbf{q}_0)$ (the latter being defined as the conditional probability density for finding a particle in the neighborhood of configuration point $\mathbf{q}$, at time t, given that it was located at $\mathbf{q}_0$ at time zero). Here, too, an estimate is made of the order of magnitude of spurious values introduced into a measurement of the scattering functions due to the finite spatial extension of the scattering system.

In summary, the following calculations have as their primary purposes: (1) a demonstration of the explicit temporal behavior of the momentum autocorrelation function for a finite system; (2) the identification of parameters determining the importance of wall perturbations occurring in measurements of the particular transport phenomena discussed above; and, (3) the estimation of the ranges of these variables for which the perturbations are significant.

II. MOMENTUM AUTOCORRELATION FUNCTION

We first investigate the temporal evolution of the momentum autocorrelation function for a one-dimensional noninteracting gas constrained by walls at which particles experience specular reflection.

The autocorrelation function $\Pi(t)$ may be obtained as follows:

$$\Pi(t) \equiv \langle \mathbf{p}(0)\cdot\mathbf{p}(t)\rangle = \int d\mathbf{p}_0\, d\mathbf{q}_0 \mathbf{p}_0 \cdot \langle \mathbf{p}; t \mid \mathbf{p}_0, \mathbf{q}_0\rangle f_0(\mathbf{p}_0, \mathbf{q}_0), \tag{2.1}$$

where $\langle \mathbf{p}; t \mid \mathbf{p}_0, \mathbf{q}_0\rangle$ is defined as the expected value of the momentum of a particle at time t, given that at $t = 0$ it had momentum $\mathbf{p}_0$ and was located at $\mathbf{q}_0$. $f_0(\mathbf{p}_0, \mathbf{q}_0)$ is the unconditioned probability density for finding a particle in the neighborhood of phase point $(\mathbf{p}_0, \mathbf{q}_0)$ at time zero.

Upon choosing a coordinate designation such that the walls are located at $q = 0$ and $q = L$ then, as a consequence of the assumption of specular reflection (by which it is meant that the collision of a particle with a wall is an instantaneous event which does not change the absolute value of the momentum of the particle), it may be readily shown that

$$\langle p; t \mid p_0, q_0\rangle = p_0^2 h_{t,q_0}(p_0), \tag{2.2}$$

where

$$h_{t,q_0} \equiv \begin{cases} +1 & \text{for } m(2nL - q_0)/t \le p_0 \\ & \quad < m([2n+1]L - q_0)/t \\ -1 & \text{for } m([2n-1]L - q_0)/t \\ & \quad \le p_0 < m(2nL - q_0)/t, \end{cases} \tag{2.3}$$

n being any integer, inclusive of zero. Consequently, upon taking the equilibrium probability density to be Maxwellian in momentum and uniform in configuration space within the box, Eq. (2.1) and Eq. (2.2) imply

$$\Pi(t) = L^{-1}\int_0^L dq_0 \int_{-\infty}^{+\infty} dp_0 p_0^2 h_{t,q_0}(p_0)\, \frac{e^{-\beta p_0^2/2m}}{(2\pi m\beta^{-1})^{\frac{1}{2}}}, \tag{2.4}$$

where $\beta^{-1} \equiv kT$.

After introducing Eq. (2.3) into the latter equation, some simple coordinate transformations provide

$$\begin{aligned}(2\pi m\beta^{-1})^{\frac{1}{2}}\Pi(t) &= \frac{1}{L}\int_{-L/2}^{+L/2} dq \left\{\left[\int_0^{Lm/2t} dp + \int_{3Lm/2t}^{5Lm/2t} dp + \cdots\right]\right. \\ &\quad \left. - \left[\int_{Lm/2t}^{3Lm/2t} dp + \int_{5Lm/2t}^{7Lm/2t} dp + \cdots\right]\right\} \\ &\quad \times \{(p - qm/t)^2 e^{-(\beta/2m)(p-qm/t)^2} \\ &\quad + (p + qm/t)^2 e^{-(\beta/2m)(p+qm/t)^2}\}. \end{aligned} \tag{2.5}$$

Next, interchange the order of the q and p integrations, and also notice that

$$\int_{-L/2}^{+L/2} dq F(q) = \int_{-\infty}^{\infty} dq F(q) H_q\left(\frac{L}{2}\right),$$

where

$$\begin{aligned} H_q(L/2) &\equiv \begin{cases} 1 & \text{if } |q| \le \tfrac{1}{2}L \\ 0 & \text{if } |q| > \tfrac{1}{2}L \end{cases} \\ &= \frac{1}{\pi}\int_{-\infty}^{+\infty} dk \frac{\sin(kL/2)}{k} e^{-ikq}. \end{aligned} \tag{2.6}$$

For example,

$$\begin{aligned}&\int_{-L/2}^{+L/2} dq (p - qm/t)^2 \exp\left[-\frac{\beta}{2m}\left(p - \frac{qm}{t}\right)^2\right] \\ &= (2\pi m\beta^{-1})^{\frac{1}{2}} \frac{t}{\pi\beta}\int_{-\infty}^{+\infty} dk \frac{\sin(kL/2)}{k}\left\{1 - \frac{k^2t^2}{\beta m}\right\} \\ &\quad \times \exp\left(-\frac{iktp}{m} - \frac{k^2t^2}{2\beta m}\right). \end{aligned} \tag{2.7}$$

Consequently, Eq. (2.5) can be expressed as

$$\Pi(t) = \frac{4m}{\pi\beta L}\sum_{n=0}^{\infty}(-1)^n\left[I_n(t) - \frac{t^2}{\beta m}\bar{I}_n(t)\right], \tag{2.8}$$

where

$$\begin{aligned} I_n(t) &\equiv \int_{-\infty}^{+\infty} dk \frac{\sin(kL/2)}{k^2}\exp\left(\frac{-k^2t^2}{2m\beta}\right) \\ &\quad \times \sin\{(n + \tfrac{1}{2})kL\} \end{aligned} \tag{2.9}$$

and

$$\tilde{I}_n(t) \equiv \int_{-\infty}^{+\infty} dk \sin(kL/2) \exp\left(\frac{-k^2t^2}{2m\beta}\right) \times \sin\{(n+\tfrac{1}{2})kL\}$$
$$= \frac{-m\beta}{t}\frac{\partial I_n}{\partial t}. \qquad (2.10)$$

Defining

$$\tilde{I} \equiv \sum_{n=0}^{\infty} (-1)^n \tilde{I}_n(t), \qquad (2.11)$$

then, by explicitly evaluating the integrals given by Eq. (2.10), it is seen that

$$\tilde{I} = \left(\frac{\beta m\pi}{2t^2}\right)^{\frac{1}{2}} \times \left\{1 + 2\sum_{n=1}^{\infty}(-1)^n \exp\left(\frac{-\beta m n^2 L^2}{2t^2}\right)\right\}. \qquad (2.12)$$

But, the term in the brackets can be identified with the zeroth theta function,[6] defined by

$$\vartheta_0(u; iv) \equiv 1 + 2\sum_{n=1}^{\infty}(-1)^n e^{-\pi v n^2}\cos(2\pi n u), \qquad (2.13)$$

so that

$$\tilde{I} = (\beta m\pi/2t^2)^{\frac{1}{2}}\vartheta_0(0; im\beta L^2/2\pi t^2). \qquad (2.14)$$

An advantage of making such an identification is that one may now make use of the following inversion formula[6]:

$$\vartheta_0(u; iv) = 1/v^{\frac{1}{2}}e^{-\pi u^2/v}\vartheta_2(iu/v; i/v), \qquad (2.15)$$

where

$$\vartheta_2(u; iv) \equiv 2\sum_{n=0}^{\infty} e^{-\pi v(n+\frac{1}{2})^2}\cos[\pi(2n+1)u]. \qquad (2.16)$$

Thus, an alternate form for Eq. (2.12) is given by

$$\tilde{I} = \frac{\pi}{L}\vartheta_2(0; i2\pi t^2/m\beta L^2) = \frac{2\pi}{L}\sum_{n=0}^{\infty}\exp\left(-\frac{2\pi^2(n+\frac{1}{2})^2t^2}{m\beta L^2}\right). \qquad (2.17)$$

We can now evaluate $I(t) \equiv \sum I_n(t)$. From Eq. (2.10),

$$I(t) = -(m\beta)^{-1}\int_0^t d\tau[\tau\tilde{I}(\tau)] + I(0), \qquad (2.18)$$

where $I(0)$ is evaluated by imposing $\Pi(0) = m/\beta$.

[6] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England 1946), 4th ed.

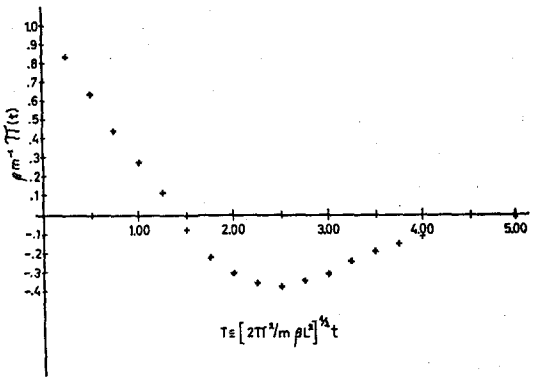

FIG. 1. Temporal evolution of the momentum autocorrelation function, as a function of the dimensionless time variable $T \equiv (2\pi^2/m\beta L^2)^{\frac{1}{2}}t$.

Hence,

$$I(t) = \frac{2\pi}{m\beta L}\sum_{n=0}^{\infty}\left\{\frac{m\beta L^2}{4\pi^2(n+\frac{1}{2})^2} \times \exp\left(\frac{-2\pi^2(n+\frac{1}{2})^2t^2}{m\beta L^2}\right)\right\}\Bigg|_0^t + \frac{\pi L}{4}$$
$$= \frac{L}{2\pi}\sum_{n=0}^{\infty}\frac{1}{(n+\frac{1}{2})^2}\exp\left(\frac{-2\pi^2(n+\frac{1}{2})^2t^2}{m\beta L^2}\right). \qquad (2.19)$$

Finally, from Eqs. (2.8), (2.10), and (2.19), the following expression for the autocorrelation function is obtained:

$$\Pi(t) = \frac{m}{\beta}\left\{\frac{2}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(n+\frac{1}{2})^2}\exp\left(\frac{-2\pi^2(n+\frac{1}{2})^2t^2}{m\beta L^2}\right) - \frac{8t^2}{m\beta L^2}\sum_{n=0}^{\infty}\exp\left(\frac{-2\pi^2(n+\frac{1}{2})^2t^2}{m\beta L^2}\right)\right\}. \qquad (2.20)$$

The rapid convergence of the representation given by Eq. (2.20) enables an explicit examination of the decay pattern of the autocorrelation function (cf. Fig. 1, where $\Pi(t)$ is plotted as a function of the reduced variable $T^2 \equiv 2\pi^2t^2/m\beta L^2$).

III. DIELECTRIC CONSTANT FOR FINITE SYSTEMS

Correlation function relations for electrical conductivities[2,3,7] may be applied to finite systems providing that boundaries constraining the motion of particles be transparent to external applied fields. Assuming, now, that the particles of the assembly carry fixed electrical charge, the frequency-dependent dielectric constant, $\epsilon(\omega)$, may be calculated as follows.

$$\epsilon(\omega) = 1 - (4\pi ne^2\beta/m^2\omega)\,\mathrm{Im}\,\chi(\omega), \qquad (3.1)$$

[7] E. W. Montroll, *Lectures in Theoretical Physics* (Boulder Lectures), Vol. III (Interscience Div., John Wiley & Sons, Inc., New York, 1961).

where n, e, and m are the density, charge, and mass, respectively, pertinent to the particles of the assembly, and ω is the frequency of the applied external field. [The Kubo relation for the dielectric constant usually appears as

$$\epsilon(\omega) = 1 - 4\pi\beta\omega^{-1} \operatorname{Im} \lim_{\lambda\to 0} \int_0^\infty dt \times \exp(i\omega - \lambda)t \langle \mathbf{J}(0)\cdot\mathbf{J}(t)\rangle = 1 - 4\pi\beta\omega^{-1} \operatorname{Im} \lim_{\lambda\to 0} \int_0^\infty dt \times \exp(i\omega - \lambda)t \sum_{i,j} \sum (e_i e_j/m_i m_j)\langle \mathbf{p}_i(0)\cdot\mathbf{p}_j(t)\rangle,$$

where $\mathbf{J}$ is the full current density due to all charge carriers of the assembly. Equation (3.2) is obtained by assuming that only one species of charged particle is the effective carrier; e.g., that a contribution due to the motion of positive ions may be neglected when compared with that due to electrons. It is to be noticed that the joint correlation terms $\langle \mathbf{p}_i(0)\cdot\mathbf{p}_j(t)\rangle$, $i \neq j$, do not appear in Eq. (3.2) since interactions between particles are ignored in our model. On the other hand, such terms could not be neglected for an interacting gas except, perhaps, if the density of charge carriers were very low.] $\chi(\omega)$ is defined by

$$\chi(\omega) = \lim_{\lambda\to 0} \int_0^\infty e^{(i\omega-\lambda)t}\Pi(t)\, dt. \tag{3.2}$$

Thus, in virtue of Eq. (2.8) and Eq. (2.10),

$$\chi(\omega) = \frac{4m}{\pi\beta L} \int_0^\infty e^{i\omega t} \frac{\partial}{\partial t}[tI(t)]\, dt = -\frac{4mi\omega}{\pi\beta L} \int_0^\infty te^{i\omega t} I(t)\, dt. \tag{3.3}$$

The latter equation implies

$$\operatorname{Im} \chi(\omega) = -\frac{4m\omega}{\pi\beta L} \frac{\partial}{\partial\omega} \int_0^\infty dt\, I(t) \sin\omega t \tag{3.4}$$

so that, upon using the explicit formula for $I(t)$ given by Eq. (2.19), one obtains

$$\operatorname{Im} \chi(\omega) = -\frac{2m\omega}{\pi^2\beta} \frac{\partial}{\partial\omega} \left\{ \frac{1}{\omega} \int_0^\infty dt \sin(t) \times \sum_{n=0}^\infty \frac{\exp[-2\pi^2(n+\frac{1}{2})^2 t^2/m\beta\omega^2L^2]}{(n+\frac{1}{2})^2} \right\}. \tag{3.5}$$

Let the infinite sum appearing in the above expression be approximated by a continuous integral:

$$\sum_{n=0}^\infty \frac{\exp[-2\pi^2(n+\frac{1}{2})^2 t^2/m\beta\omega^2L^2]}{(n+\frac{1}{2})^2} \approx k \int_0^\infty dx \frac{\exp[-2\pi^2(x+\frac{1}{2})^2 t^2/m\beta\omega^2L^2]}{(x+\frac{1}{2})^2},$$

where k, a constant, is to be determined such that the sum has the correct value for $\omega L \to \infty$ (i.e., $\sum_{n=0}^\infty (n+\frac{1}{2})^{-2} = k \int_{\frac{1}{2}}^\infty dx/x^2$).

Clearly, $k = \pi^2/4$.

Under such an approximation, Eq. (3.5) becomes

$$\operatorname{Im} \chi(\omega) \approx -\frac{m\omega}{2\beta} \frac{\partial}{\partial\omega} \left\{ \frac{1}{\omega} \int_{\frac{1}{2}}^\infty dx \int_0^\infty dt \sin(t) \times \frac{\exp(-2\pi^2x^2t^2/m\beta\omega^2L^2)}{x^2} \right\} = -\frac{m\omega}{\beta} \frac{\partial}{\partial\omega} \left\{ \frac{1}{\omega} \int_{\frac{1}{2}}^\infty \frac{dx}{x^2} \int_0^{m\beta\omega^2L^2/8\pi^2x^2} d\eta \times \eta \left[1 - \frac{8\pi^2x^2\eta^2}{m\beta\omega^2L^2}\right]^{\frac{1}{2}} e^{-\eta^2} \right\}. \tag{3.6}$$

Let us examine the latter expression when $\omega L \gg 1$. First, it is to be noticed that

$$\lim_{L\to\infty} \chi(\omega) = -\frac{m\omega}{\beta} \frac{\partial}{\partial\omega} \left\{ \frac{1}{\omega} \int_{\frac{1}{2}}^\infty \frac{dx}{x^2} \int_0^\infty \eta e^{-\eta^2} d\eta \right\} = \frac{m}{\beta\omega}, \tag{3.7}$$

which is the correct limit for a gas of noninteracting particles. On the other hand, as an approximation for large but finite ωL,

$$\operatorname{Im} \chi(\omega) \approx -\frac{m\omega}{\beta} \frac{\partial}{\partial\omega} \left\{ \frac{1}{\omega} \int_{\frac{1}{2}}^\infty \frac{dx}{x^2} \times \int_0^{m\beta L^2\omega^2/8\pi^2x^2} \eta e^{-\eta^2} d\eta \right\} \tag{3.8}$$

$$= -\frac{m\omega}{\beta} \frac{\partial}{\partial\omega} \left\{ \frac{1}{\omega} \left[1 - \left(2\frac{\pi^2}{m\beta L^2\omega^2}\right)^{\frac{1}{2}} \times \int_0^{2(m\beta L^2\omega^2/8\pi^2)^{\frac{1}{2}}} e^{-y^2} dy \right] \right\} \approx (m/\beta\omega)\{1 - (2\pi^3)^{\frac{1}{2}}(m\beta\omega^2L^2)^{-\frac{1}{2}}\}. \tag{3.9}$$

Comparing Eq. (3.9) with Eq. (3.7), it is seen that for large but finite ωL, the measured dielectric constant, $[\epsilon(\omega) - 1]$, will be diminished by a quantity which is inversely proportional to $(m\beta\omega^2L^2)^{\frac{1}{2}}$. In virtue of Eq. (3.9), it may be concluded that boundary effects will be unimportant if $m\beta\omega^2L^2 \gg 10^2$.[8] [These conditions are certainly met *a propos* microwave analysis of plasmas, even if the plasma is quite hot. (Assume $L \approx 1$ cm, $T \approx 30\,000$°K, $\omega \approx 10^{10}$ cps. Since the electron mass $\approx 10^{-27}$ gm, one has $m\beta\omega^2L^2 \approx 10^4 \gg 10^2$.) On the other hand,

[8] An investigation of $\chi(\omega)$ for small (ωL) appears in Appendix A, below.

analysis at radio frequency would be complicated by boundary effects. (Even if $L \approx 10$ cm and $T \approx 300°\text{K}$, because $\omega \approx 10^7$ cps one would have $m\beta\omega^2L^2 \approx 10^2$, so that the inequality would not be satisfied.)]

IV. SCATTERING FUNCTIONS

Let us next consider certain functions appearing in the scattering theory of slow neutrons.[4,5] The same model as that employed in the calculation of the momentum autocorrelation function (cf. Sec. II) is used in the following analysis.

First, consider the time-relaxed spatial density, $G_s(\mathbf{q}; t \mid \mathbf{q}_0)$, defined as the conditional probability density for finding a particle in the neighborhood of phase point $\mathbf{q}$, at time t, given that it was located at $\mathbf{q}_0$ at time zero. This function can be obtained from

$$G_s(\mathbf{q}; t \mid \mathbf{q}_0) = \iint d\mathbf{p}\, d\mathbf{p}_0 \frac{\exp(-\beta\mathbf{p}_0^2/2m)}{(2\pi m\beta^{-1})^{\frac{1}{2}}} \times f(\mathbf{p}, \mathbf{q}; t \mid \mathbf{p}_0, \mathbf{q}_0)$$
$$= \int d\mathbf{p}_0 \frac{\exp(-\beta\mathbf{p}_0^2/2m)}{(2\pi m\beta^{-1})^{\frac{1}{2}}} \times f(\mathbf{q}; t \mid \mathbf{p}_0, \mathbf{q}_0), \quad (4.1)$$

where $f(\mathbf{q}; t \mid \mathbf{p}_0, \mathbf{q}_0)$ is the conditional probability density for finding a particle in the neighborhood of $\mathbf{q}$, at time t, given that at $t = 0$ it was located at $\mathbf{q}_0$ and had momentum $\mathbf{p}_0$.

However,

$$f(\mathbf{q}; t \mid \mathbf{p}_0, \mathbf{q}_0) = \delta(\mathbf{q} - \mathbf{q}(t \mid \mathbf{p}_0, \mathbf{q}_0)) \quad (4.2)$$

where $\mathbf{q}(t \mid \mathbf{p}_0, \mathbf{q}_0)$ is the position of a particle at time t, given that at $t = 0$ it was located at $(\mathbf{q}_0, \mathbf{p}_0)$. It is to be recognized that the latter is given by

$$q(t \mid p_0, q_0) = \begin{cases} \left(q_0 + \dfrac{p_0 t}{m} - 2nL\right) & \text{for } \dfrac{2nmL}{t} - \dfrac{q_0 m}{t} < p_0 \leq \dfrac{(2n+1)mL}{t} - \dfrac{q_0 m}{t} \\ -\left(q_0 + \dfrac{p_0 t}{m} - 2nL\right) & \text{for } \dfrac{(2n-1)mL}{t} - \dfrac{q_0 m}{t} < p_0 \leq \dfrac{2nmL}{t} - \dfrac{q_0 m}{t} \end{cases}$$
$$n = \cdots, -2, -1, 0, 1, 2, 3, \cdots. \quad (4.3)$$

Upon placing Eq. (4.3) into Eq. (4.1) and performing some simple coordinate transformations, it may be readily shown that

$$G_s(q; t \mid q_0) = \sum_{n=0}^{\infty} \int_0^{Lm/t} dp\, g[p + 2nmL/t \mid q_0]\delta(q - pt/m) + \sum_{n=0}^{\infty} \int_0^{Lm/t} dp\, g[p + (2n+1)mL/t \mid q_0] \times \delta(q + [pt/m - L]), \quad (4.4)$$

where

$$g(p \mid q) \equiv (2\pi m\beta^{-1})^{-\frac{1}{2}} \times \{e^{-(\beta/2m)(p+q_0m/t)^2} + e^{-(\beta/2m)(p-q_0t/m)^2}\}. \quad (4.5)$$

Let us now discuss the relationship of G_s to the scattering theory of slow neutrons. The cross section for the scattering of low-energy neutrons may be expressed as

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \frac{1}{4\pi\hbar}\frac{K'}{K_0}[a_{\text{coh}}^2 S_{\text{coh}}(k, \omega) + a_{\text{inc}}^2 S_{\text{inc}}(k, \omega)], \quad (4.6)$$

where $S_{\text{coh}}(k, \omega)$ and $S_{\text{inc}}(k, \omega)$ are referred to as the coherent and incoherent scattering functions, respectively.[9] We focus our attention on the second of these, which has the following definition.[4]

$$S_{\text{inc}}(k, \omega) \equiv \int_{-\infty}^{+\infty} dt\, e^{-i\omega t}\chi_s(k, t) \quad (4.7)$$

with

$$\chi_s(k, t) \equiv \frac{1}{N}\sum_j \langle \exp[-ik\cdot q_j(0)] \exp[+ik\cdot q_j(t)]\rangle_T. \quad (4.8)$$

In the approximation of classical mechanics, the joint expectation defined by Eq. (4.8) has the following interpretation:

$$\chi_s(k, t) = \int dq_0\, P(q_0) \int dq\, e^{ik\cdot(q-q_0)} P(q \mid q_0), \quad (4.8')$$

with $P(q \mid q_0)$ being the probability density for finding a particle in the neighborhood of q at time t, given that it was at q_0 at $t = 0$; $P(q_0)$ is the unconditioned probability density for finding the particle in the neighborhood of q_0 at $t = 0$.

Thus, in the classical approximation, and within

[9] a_{coh} and a_{inc} are, respectively, the coherent and incoherent scattering lengths. $\mathbf{K}_0$ and $\mathbf{K}'$ are the wavenumbers of the neutron before and after scattering; $\mathbf{k} \equiv \mathbf{K}_0 - \mathbf{K}'$.

the approximations of the model used for this calculation, the incoherent scattering function can be expressed as

$$S_{\text{inc}}(k, \omega) = L^{-1} \int_0^L dq_0 S(k, \omega \mid q_0), \tag{4.9}$$

where

$$S(k, \omega \mid q_0) \equiv \int_{-\infty}^{+\infty} dt e^{-i\omega t} \chi(k, t \mid q_0), \tag{4.10}$$

and

$$\chi(k, t \mid q_0) \equiv \int_{-\infty}^{+\infty} dq e^{ik(q-q_0)} G(q; t \mid q_0). \tag{4.11}$$

The effects of boundaries on a measurement of $S_{\text{inc}}(k, \omega)$ may now be estimated. From Eq. (4.5) and Eq. (4.11) one immediately obtains

$$\begin{aligned}\chi(k, t \mid q_0) &= \sum_{n=0}^{\infty} \int_0^{Lm/t} dp\, g(p + 2nmL/t \mid q_0) e^{i(pt/m - q_0)k} \\ &+ \sum_{n=0}^{\infty} \int_0^{Lm/t} dp\, g(p + [2n+1]mL/t \mid q_0) \\ &\times e^{-i(q_0 + pt/m - L)k}.\end{aligned} \tag{4.12}$$

Consequently, in virtue of Eq. (4.5),

$$\begin{aligned}(2\pi m\beta^{-1})^{\frac{1}{2}} \chi(k, t \mid q_0) &= \frac{2m}{t} \sum_{n=1}^{\infty} \Bigg[\int_0^L dp \\ &\times \left\{ \cosh\left(\frac{2\beta nmL}{t^2}[p + q_0]\right) e^{-(\beta m/2t^2)(p+q_0)^2} \right. \\ &\left. + \cosh([2\beta nmL/t^2][p - q_0]) e^{-(\beta m/2t^2)(p-q_0)^2} \right\} \\ &\times e^{-2\beta mn^2L^2/t^2} e^{i(p-q_0)k} \Bigg] + \frac{m}{t} \int_0^L dp \\ &\times \{ e^{-(\beta m/2t^2)(p+q_0)^2} + e^{-(\beta m/2t^2)(p-q_0)^2} \} e^{i(p-q_0)k},\end{aligned} \tag{4.13}$$

where, in order to obtain Eq. (4.13) it has been noticed that

$$e^{-(A+B)^2} + e^{-(A-B)^2} = 2e^{-A^2} e^{-B^2} \cosh 2AB.$$

Again using the Fourier representation for the step function [cf. Eq. (2.6) and ff.], one obtains

$$\begin{aligned}(2\pi m\beta^{-1})^{\frac{1}{2}} \chi(k, t \mid q_0) &= \frac{4m}{t} \sum_{n=1}^{\infty} \Bigg[\int_{-\infty}^{+\infty} d\theta \frac{\sin(\theta L/2)}{\pi\theta} e^{i\theta L/2} \\ &\times \int_{-\infty}^{+\infty} dp \{ e^{-i\theta p} e^{-2\beta m(n^2L^2 + \frac{1}{4}p^2)/t^2} \\ &\times \cos(2\beta nmLp/t^2) \\ &\times \cos([k - \theta]q_0) e^{i(p-q_0)k} \} \Bigg] \\ &+ \frac{2m}{t} \int_{-\infty}^{+\infty} d\theta \frac{\sin(\theta L/2)}{\pi\theta} e^{i\theta L/2} \\ &\times \int_{-\infty}^{+\infty} dp\, e^{-(\beta mp^2/2t^2 + i\theta p - i[p-q_0]k)} \\ &\times \cos([k - \theta]q_0).\end{aligned} \tag{4.14}$$

However, let it be recalled that the theta function of the third kind is defined by[6]

$$\vartheta_3(u; iv) = 1 + 2 \sum_{n=1}^{\infty} e^{-\pi v n^2} \cos(2\pi nu). \tag{4.15}$$

With this identification, Eq. (4.14) yields, simply,

$$\begin{aligned}&(2\pi m\beta^{-1})^{\frac{1}{2}} \chi(k, t \mid q_0) \\ &= \frac{2m}{t} \int_{-\infty}^{+\infty} d\theta \frac{\sin(\theta L/2)}{\pi\theta} e^{i\theta L/2} \\ &\times \int_{-\infty}^{+\infty} dp \{ e^{-i\theta p} e^{-\beta mp^2/2t^2} \cos([k - \theta]q_0) \\ &\times \vartheta_3(i\beta Lmp/\pi t^2; 2i\beta mL^2/\pi t^2) e^{i(p-q_0)k} \}.\end{aligned} \tag{4.16}$$

An advantage of making the identification given by Eq. (4.15) is that one can now make use of well-known expansions of the ϑ functions in order to facilitate evaluation of asymptotic expressions for the scattering functions. Indeed, the Jacobi factorization for ϑ_3 is given by[6]

$$\begin{aligned}\vartheta_3(u; iv) = F \prod_{n=1}^{\infty} [1 &+ 2e^{-(2n-1)\pi v} \\ &\times \cos(2\pi u) + e^{-(4n-2)\pi v}],\end{aligned} \tag{4.17}$$

where

$$F \equiv \prod_{n=1}^{\infty} (1 - e^{-2n\pi v}).$$

Thus, in virtue of Eq. (4.17), Eq. (4.16), and Eq. (4.10),

$$\begin{aligned}&(2\pi m\beta^{-1})^{\frac{1}{2}} S(k, \omega \mid q_0) \\ &= 2m \int_{-\infty}^{+\infty} dt \frac{e^{-it}}{t} \int_{-\infty}^{+\infty} d\theta \frac{\sin\theta/2}{\pi\theta} e^{i\theta/2} \\ &\times \int_{-\infty}^{+\infty} dp \Big\{ e^{-i\theta p/L} e^{-\beta mp^2\omega^2/2t^2} \\ &\times \cos([k - \theta/L]q_0) e^{i(p-q_0)k} \\ &\times \prod_{\tilde{n}=1}^{\infty} [1 - \exp(-4\tilde{n}\beta mL^2\omega^2/t^2)] \\ &\times \prod_{n=1}^{\infty} [1 + 2\exp(-[4n-2]\beta mL^2\omega^2/t^2) \\ &\times \cosh(2\beta mL\omega^2 p/t^2) \\ &+ \exp(-[8n-4]\beta mL^2\omega^2/t^2)] \Big\}.\end{aligned} \tag{4.18}$$

However, for $\beta m L^2\omega^2 \gg 1$,

$$
\begin{aligned}
&(2\pi m\beta^{-1})^{\frac{1}{2}} S(k,\omega \mid q_0) \\
&\quad \approx 2m \int_{-\infty}^{+\infty} dt \frac{e^{-it}}{t} \int_{-\infty}^{+\infty} d\theta \frac{\sin\theta/2}{\pi\theta} e^{i\theta/2} \\
&\qquad \times \int_{-\infty}^{+\infty} dp \{ e^{-i\theta p/L} e^{-\beta m p^2\omega^2/2t^2} \\
&\qquad \times \cos([k - \theta/L]q_0) e^{i(p-q_0)k} \\
&\qquad \times [1 + 2\exp(-2\beta m L^2\omega^2/t^2) \\
&\qquad \times \cosh(2\beta m L\omega^2 p/t^2)]\}, \qquad (4.19)
\end{aligned}
$$

the latter approximation being valid due to the fact that for large t, where the neglected terms of the product factorization would be important, the decreasing multiplicative factor, e^{-it}/t, becomes dominantly small.

Performing the q_0 integration which is necessary in order to obtain $S(k, \omega)$ from $S(k, \omega \mid q_0)$ [cf. Eq. (4.9)], Eq. (4.19) yields

$$
\begin{aligned}
&(2\pi m\beta^{-1}) S_{\text{inc}}(k,\omega) = 2m \int_{-\infty}^{+\infty} dt\, e^{-it}/t \int_{-\infty}^{+\infty} d\theta \\
&\times \left\{ \frac{\sin(\theta/2)}{\pi\theta} e^{i\theta/2} \frac{1}{2i} \left[\frac{(1 - e^{-i\theta})}{\theta} + \frac{(1 - e^{-i(2kL-\theta)})}{(2kL - \theta)} \right] \right. \\
&\left. \times \int_{-\infty}^{+\infty} dp\, e^{-i\theta(p/L-k)} e^{-m\beta\omega^2 p^2/2t^2} \right\} \\
&+ 2m \int_{-\infty}^{+\infty} dt \frac{e^{-it}}{t} \int_{-\infty}^{+\infty} d\theta \left\{ \frac{\sin(\theta/2)}{\pi\theta} e^{i\theta/2} \cdot \frac{1}{2i} \right. \\
&\times \left[\frac{(1 - e^{-i\theta})}{\theta} + \frac{(1 - e^{-i(2kL-\theta)})}{(2kL - \theta)} \right] \\
&\times \int_{-\infty}^{+\infty} dp\, e^{-i\theta(p/L-k)} [e^{-m\beta\omega^2(p-2L)^2/2t^2} \\
&\left. + e^{-m\beta\omega^2(p+2L)^2/2t^2}] \right\}. \qquad (4.20)
\end{aligned}
$$

Finally, as shown in Appendix B, careful analysis of the latter (for $kL \gg 1$) yields

$$
\begin{aligned}
&S_{\text{inc}}(k,\omega) = \left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}} e^{-m\beta\omega^2/2k^2} \\
&\times \left[1 + \frac{f(k)}{|kL|} + o\left(\frac{1}{(kL)^2} ; \frac{1}{kL} \frac{1}{(m\beta\omega^2 L^2)^{\frac{1}{2}}} \right) + \cdots \right], \qquad (4.21)
\end{aligned}
$$

with

$$
|f(k)| \equiv 4\,|\cos^3(kL)\sin(kL)| \leq 4. \qquad (4.22)
$$

The leading term in Eq. (4.21) is that appropriate to an unconstrained one-dimensional noninteracting gas, whereas the term proportional to $(kL)^{-1}$ provides the first-order correction.

In scattering experiments, detectable energy changes are usually of the order $\hbar\omega > 0.001$ eV. Corresponding to such an energy change,[5] $k^{-1} = .287 \times 10^{-8}/(E_{\text{ev}})^{\frac{1}{2}} \lesssim 10^{-7}$ cm. Thus, for realistic experimental conditions, boundary effects are unlikely to be of any important concern.

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APPENDIX A: DIELECTRIC CONSTANT FOR SMALL (ωL)

Let us briefly investigate $\chi(\omega)$ for values of $(\beta m\omega^2 L^2) \sim o(1)$. Starting with Eq. (3.5), integration over t provides

$$
\begin{aligned}
\text{Im}\,\chi(\omega) &= \frac{m\omega}{\pi^2\beta} \left\{ \sum_{n=0}^{\infty} \frac{\omega^2}{2} \left[\frac{m\beta L^2}{2\pi^2(n + \frac{1}{2})^2} \right]^2 \right. \\
&\quad \times \int_0^1 \exp\left[-\frac{m\beta L^2\omega^2}{8\pi^2(n + \frac{1}{2})^2} (1 - y^2) \right] dy \\
&\quad \left. - \sum_{n=0}^{\infty} \frac{m\beta L^2}{2\pi^2(n + \frac{1}{2})^2} \right\}. \qquad (A1)
\end{aligned}
$$

However, for small $L\omega$, the integrals appearing in the above equation may be approximated by unity. In this case,

$$
\begin{aligned}
&\text{Im}\,\chi(\omega) \\
&\quad \approx (m/4\pi^2\beta\omega)\{m\beta L^2\omega^2\}\{\tfrac{1}{6}(m\beta L^2\omega^2) - 1\}. \qquad (A2)
\end{aligned}
$$

Hence, in the rf range, $\chi(\omega)$ would have a sign change as a function of frequency.

APPENDIX B: ASYMPTOTIC ANALYSIS

The expression given by Eq. (4.20) may be written as

$$
S_{\text{inc}}(k,\omega) = [S_1 + S_2] + [S_3 + S_4], \qquad (B1)
$$

where

$$
\begin{aligned}
&(2\pi m\beta^{-1})^{\frac{1}{2}} S_1 \equiv 2m \int_{-\infty}^{+\infty} dt \frac{e^{-it}}{t} \\
&\qquad \times \int_{-\infty}^{+\infty} d\theta \frac{[\sin\theta/2] e^{i\theta/2}}{2i\pi\theta^2} (1 - e^{-i\theta}) \\
&\qquad \times \int_{-\infty}^{+\infty} dp\, e^{-i\theta(p/L-k)} e^{-m\beta p^2\omega^2/2t^2} \qquad (B2)
\end{aligned}
$$

$$
\begin{aligned}
&(2\pi m\beta^{-1})^{\frac{1}{2}} S_2 \equiv 2m \int_{-\infty}^{+\infty} dt \frac{e^{-it}}{t} \\
&\times \int_{-\infty}^{+\infty} d\theta \frac{[\sin\theta/2] e^{i\theta/2}}{2i\pi\theta(2kL - \theta)} (1 - e^{-i(2kL-\theta)}) \\
&\times \int_{-\infty}^{+\infty} dp e^{-i\theta(p/L-k)} e^{-m\beta p^2\omega^2/2t^2}, \qquad (B3)
\end{aligned}
$$

$$(2\pi m\beta^{-1})^{\frac{1}{2}}S_3 \equiv 2m\int_{-\infty}^{+\infty} dt\,\frac{e^{-it}}{t} \times \int_{-\infty}^{+\infty} d\theta\,\frac{[\sin\theta/2]e^{i\theta/2}}{2i\pi\theta^2}(1-e^{-i\theta}) \times \int_{-\infty}^{+\infty} dp e^{-i\theta(p/L-k)} \times [e^{-(\beta m\omega^2/2t^2)(p+2L)^2} + e^{-(\beta m\omega^2/2t^2)(p-2L)^2}] \tag{B4}$$

and

$$(2\pi m\beta^{-1})^{\frac{1}{2}}S_4 \equiv 2m\int_{-\infty}^{+\infty} dt\,\frac{e^{-it}}{t} \times \int_{-\infty}^{+\infty} d\theta\,\frac{[\sin\theta/2]e^{i\theta/2}[1-e^{-i(2kL-\theta)}]}{2i\pi\theta(2kL-\theta)} \times \int_{+\infty}^{+\infty} dp e^{-i\theta(p/L-k)}[e^{-(\beta m\omega^2/2t^2)(p+2L)^2} + e^{-(\beta m\omega^2/2t^2)(p-2L)^2}]. \tag{B5}$$

Let us analyze each one of these terms separately.

Noticing that $[e^{i\theta/2}(1-e^{-i\theta})]/2i = \sin(\theta/2)$, the first contribution may be written as

$$S_1 = \left(\frac{\beta}{2\pi m}\right)^{\frac{1}{2}}\left\{2m\int_{-\infty}^{+\infty} dt\,\frac{e^{-it}}{t}\int_{-\infty}^{+\infty} d\theta\,\frac{\sin^2(\theta/2)}{\pi\theta^2} \times \sum_{n=0}^{\infty}\frac{1}{(2n)!}\left(\frac{\theta}{L}\frac{\partial}{\partial k}\right)^{2n}\int_{-\infty}^{+\infty} dp\,e^{-m\beta p^2\omega^2/2t^2}\cos(pk)\right\} \tag{B6}$$

$$= \int_{-\infty}^{+\infty} d\theta\left\{\frac{2\sin^2(\theta/2)}{\pi\theta^2}\sum_{n=0}^{\infty}\frac{1}{(2n)!}\left(\frac{\theta}{L}\frac{\partial}{\partial k}\right)^{2n}\right\} \times \left\{\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2}\right\}$$

$$= (2\pi m\beta/k^2)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2}[1-o(1/k^2L^2)+\cdots]. \tag{B6'}$$

Similarly, as a consequence of the coordinate transformation $\phi \equiv \theta - kL$, one obtains (for $|kL| \gg 1$)

$$S_2 = \left(\frac{\beta}{2\pi m}\right)^{\frac{1}{2}}\int_{-\infty}^{+\infty} d\phi\,\frac{2e^{-i\varphi}}{\pi} \times \frac{\sin(\frac{1}{2}\varphi-\frac{1}{2}kL)\sin(\frac{1}{2}\varphi+\frac{1}{2}kL)}{(\varphi-kL)(\varphi+kL)}\frac{(2\pi mL)}{|\varphi|}e^{-m\beta\omega^2L^2/2\varphi^2} \tag{B7}$$

$$\approx 2\cos(kL)\frac{\sin(kL)}{|kL|}\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2} \times \int_{-\infty}^{+\infty} d\varphi\,\frac{\sin([\varphi-|k|\,L]/2)}{\pi(\varphi-|k|\,L)} + 2\frac{\sin^2(kL/2)}{|kL|}\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}} \times \int_{-\infty}^{+\infty} d\varphi\,\frac{e^{-i\varphi}}{\pi\,|\varphi|}e^{-m\beta\omega^2L^2/2\varphi^2}$$

$$= 2\cos(kL)\frac{\sin(kL)}{|kL|}\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2} + o\left(\frac{1}{kL}\frac{1}{[m\beta\omega^2L^2]^{\frac{1}{2}}}\right). \tag{B7'}$$

For the third term,

$$S_3 = 4\int_{-\infty}^{+\infty} d\theta\left[\frac{\sin^2(\theta/2)}{\pi\theta^2}\sum_{n=0}^{\infty}\frac{1}{(2n)!}\left(\frac{\theta}{L}\frac{\partial}{\partial k}\right)^{2n}\right] \times \left\{\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}\cos(2kL)e^{-m\beta\omega^2/2k^2}\right\} \tag{B8}$$

$$= 4\int_{-\infty}^{+\infty} d\theta\left[\frac{\sin^2(\theta/2)}{\pi\theta^2}\cos 2\theta\right] \times \left\{\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}\cos 2kL\,e^{-m\beta\omega^2/2k^2}\right\} + 2\int_{-\infty}^{+\infty} d\theta\left[\frac{\sin^2(\theta/2)}{\pi\theta}\sin 2\theta\right] \times \left\{\sin 2kL\cdot\frac{1}{L}\frac{\partial}{\partial k}\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2}\right\} + o\left(\frac{1}{k^2L^2}\right)\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2}+\cdots. \tag{B8'}$$

But[10]

$$\int_{-\infty}^{+\infty} d\theta\,\frac{\sin^2(\theta/2)}{\theta^2}\cos 2\theta = 0, \qquad \int_{-\infty}^{+\infty} d\theta\,\frac{\sin^2(\theta/2)}{\theta}\sin 2\theta = 0. \tag{B9}$$

Hence, S_3 is at most only of order $1/k^2L^2$ of the strength of S_1.

Finally, from Eq. (B5),

$$S_4 = \int_{-\infty}^{+\infty} d\theta\left\{\frac{2e^{-i\theta}}{\pi}\frac{\sin([\theta-kL]/2)\sin([\theta+kL]/2)}{(\theta-kL)(\theta+kL)} \times [2\cos 2\theta][(2\pi m\beta)^{\frac{1}{2}}L/|\theta|]e^{-m\beta\omega^2L^2/2\theta^2}\right\} \tag{B10}$$

$$\approx 2\frac{\cos 2kL}{|kL|}\sin(kL)\cos(kL) \times \int_{-\infty}^{+\infty} d\theta\,\frac{\sin\theta}{\pi\theta}\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2} + o\left(\frac{1}{kL}\frac{1}{(m\beta\omega^2L^2)^{\frac{1}{2}}}\right)$$

$$\approx 2\left[\frac{\cos 2kL}{|kL|}\cos(kL)\sin(kL)\right] \times \left\{\left(\frac{2\pi m\beta}{k^2}\right)^{\frac{1}{2}}e^{-m\beta\omega^2/2k^2}\right\}. \tag{B10'}$$

Thus, by virtue of Eqs. (B10), (B7'), and (B6'), Eq. (B1) implies Eq. (4.21) of the main text.

[10] H. B. Dwight, *Tables of Integrals and Other Mathematical Data* (The Macmillan Company, New York, 1961), 4th ed.

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Correlation Functionals

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The correlations between positions of particles in classical equilibrium statistical mechanics are usually expressed by correlation functions. It can be seen that if the correlation functions of a system are known, its configurational entropy per unit volume is already determined (independently of the interaction potential or other thermodynamical parameters). In this paper we consider all sequences of functions of an increasing number of variables (these functions are candidates for correlation functions) for which an entropy per unit volume may be defined. These sequences are called correlation functionals and are investigated in detail. They prove useful to the study of the limit of an infinite system in statistical mechanics (thermodynamic limit). Furthermore they allow the segregation of certain thermodynamic systems into phases to be made evident.

INTRODUCTION

STRIPPED of its unessential features, the main problem of equilibrium statistical mechanics is typically the following. Given a large box Λ with volume V and a large number n of particles enclosed in the box and interacting through a two-body potential Φ, what is the macroscopic aspect of the system of particles? We assume that the density d and the energy per unit volume e are given, then (forgetting kinetic energy) every admissible configuration $(\mathbf{x}_1, \cdots, \mathbf{x}_n)$ of the particles in the box satisfies the conditions

$$V^{-1}n = V^{-1}\sum_{i=1}^{n} 1 \approx d, \quad V^{-1}\sum_{i<j} \Phi(x_i - x_j) \approx e. \quad (0.1)$$

We ignore configurations with "exceptional" behavior, sets of configurations being weighted with Lebesgue measure. According to the usual ideas about ergodicity, and from the existence of thermodynamics, one is led to think that the problem described above is reasonably well set (for reasonable Φ).

In the greater part of this paper, the configurations satisfying conditions of the type (0.1) are studied without further reference to physics. In the last two sections, applications to equilibrium statistical mechanics are indicated, without attempt to generality. In Secs. 1 to 3 the limit of an infinite volume V is investigated, using methods analogous to those employed by the author[1] and Fisher[2] to prove the existence of the thermodynamic limit, generalizing the classical result of Lee and Yang.[3] In Secs. 4 to 6 the notion of correlation functionals is defined and studied. In Secs. 7 to 9, correlation functionals are represented in terms of expectation values in a Hilbert space, in a manner which is reminiscent of quantum field theory. A notion of analytic correlation functional is introduced. In Sec. 10, the preceding theory is applied to the study of the thermodynamic limit of the grand canonical correlation functions. In Sec. 11, a (unique) decomposition of analytic correlation functionals, established in Sec. 9, is shown to correspond to a physical splitting of large systems into *phases*.

Throughout the paper we have, in a somewhat pedantic way, distinguished between a real Lebesgue-measurable function $\tilde{A}$ and its class A. It is assumed that the irritated reader will mentally omit the tilde. Furthermore systematic use has been made of symbols like N^* [to represent the set of positive or rather, as one should say, *strictly* positive (>0) integers]. The text has been written so that it is possible to go through Sec. 1, Sec. 7 and only the italicized part (definitions, propositions, theorems) of the other sections and to get, in this way, rapidly an idea of the results obtained in the paper. This also gives quick access to the motivation which is contained in the last two sections.

The main results of physical interest may however already be stated now, although in an imprecise manner. A correlation functional ρ is defined as a sequence of functions of an increasing number of variables: $\rho = (\rho_1, \rho_2(\xi_1), \rho_3(\xi_1, \xi_2), \cdots)$. In such a sequence the function $\rho_{p+1}(\xi_1, \cdots \xi_p)$ may be understood as the probability density of finding $p + 1$ *different* particles at positions $x, x + \xi_1, \cdots, x + \xi_p$ (ρ_{p+1} is thus a candidate for a correlation function in statistical mechanics). To each ρ we will further attach a real number $s(\rho)$, its entropy per unit volume. Consider a sequence (Λ_j) of boxes of volumes

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[1] D. Ruelle, Helv. Phys. Acta **36**, 183 (1963) and Lecture notes of the Theoretical Physics Institute, University of Colorado, Boulder, Summer 1963.
[2] M. Fischer, Arch. Ratl. Mech. Anal. (to be published).
[3] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952).

V_i tending to infinity and let $\mathfrak{u}_i$ be the volume of the set of configurations of points in V_i, the correlations of which are given (in the limit) by ρ. The entropy per unit volume of ρ is defined as

$$s(\rho) = \lim_{i\to\infty} V_i^{-1} \log \mathfrak{u}_i. \tag{0.2}$$

The existence of the limit (0.2) is not trivial and is a central result of the paper.

We show that, for potentials of a certain type at least (hard-core potentials), if we compute the grand canonical correlation functions at any given temperature and chemical potential for a sequence of boxes tending to infinity, we can choose a subsequence of the sequence of boxes such that the correlation functions have limits, which form a correlation functional ρ. Furthermore $s(\rho)$ is the physical entropy per unit volume. This result justifies the names given to ρ and $s(\rho)$. The idea here is the following. Suppose that some correlations are fixed for a large system of points [by such conditions as (0.1)]. If a new correlation condition is imposed it may or may not decrease the entropy per unit volume of the system. If it does, that new condition is inadequate because it leads to a set of configurations which has negligible probability; if it doesn't, we proceed by imposing new correlation conditions. In this way, one can find which correlation functionals, compatible with the original correlation conditions, have the same entropy per unit volume, and may therefore describe the system.

For a large class of correlation functionals there exists a natural and unique decomposition into a sum (or integral) of similar objects. This is true in particular for analytic correlation functionals (which justifies their introduction). This decomposition is seen to correspond to a decomposition of a physical system into phases, defined as large, macroscopically homogeneous, regions. A short heuristic discussion of how phase transitions may occur is given at the end of Sec. 11.

1. NOTATIONS AND BASIC INEQUALITIES

Let R be the field of real numbers and Z the ring of integers. It will be convenient in what follows to use systematically the notations

$$R_+ = \{x : x \in R, x \geq 0\},$$
$$R_+^* = \{x : x \in R, x > 0\},$$
$$N = \{n : n \in Z, n \geq 0\},$$
$$N^* = \{n : n \in Z, n > 0\}.$$

Let R^ν be the ν-dimensional numerical space, $\nu \in N^*$, with the usual topology. An element x of R^ν is a sequence $(x^i)_{1\leq i\leq \nu}$ of real numbers and we write $x_0 = x_1 + x_2$ if $x_0^i = x_1^i + x_2^i$ for $i = 1, 2, \cdots, \nu$. A translation τ_{x_0}, $x_0 \in R^\nu$ is the mapping of R^ν onto itself defined by

$$\tau_{x_0} x = x + x_0. \tag{1.1}$$

It will be understood in what follows that the measure of a subset of R^ν is its Lebesgue measure (volume); measurability will mean Lebesgue measurability.

We will call $\mathfrak{A}_{p+1}$, $p \in N^*$, the set of all measurable functions defined on $R^{p\nu}$, with values in $R \cup \{+\infty\}$, and vanishing outside of a bounded set. We call $\mathfrak{a}_{p+1}$ the set of classes of such functions (two functions are said to belong to the same class if they differ only on a set of measure zero). We will denote by $(\xi_1, \cdots, \xi_p)$, with $\xi_1, \cdots, \xi_p \in R^\nu$, a point of $R^{p\nu}$, and by $\tilde{A}_{p+1}(\xi_1, \cdots, \xi_p)$ the value of $\tilde{A}_{p+1}$ at this point. We also let $\mathfrak{A}_1$ and $\mathfrak{a}_1$ be identical with R and say that $\tilde{A}_1 \in \mathfrak{A}_1$ belongs to the class of $A_1 \in \mathfrak{a}_1$ if $\tilde{A}_1 = A_1 \in R$. Let $\tilde{A} = (\tilde{A}_{p+1})_{p\in N}$ be a sequence such that, for each $p \in N$, $\tilde{A}_{p+1} \in \mathfrak{A}_{p+1}$ and only a finite number of terms in the sequence do not vanish. We call $\mathfrak{A}$ the set of all such sequences $\tilde{A}$. We say that a sequence $A = (A_{p+1})_{p\in N}$ is the class of an element $\tilde{A} = (\tilde{A}_{p+1})_{p\in N}$ of $\mathfrak{A}$ if, for each $p \in N$, $A_{p+1} \in \mathfrak{a}_{p+1}$ is the class of $\tilde{A}_{p+1}$. We call $\mathfrak{a}$ the set of all such sequences A.

Let $\mathfrak{R}$ be the topological sum,[4] for $p \in N$, of the spaces $R^{p\nu}$. We make use on $\mathfrak{R}$ of the measure which reduces on $R^{p\nu}$ to the Lebesgue measure for $p \in N^*$ and to 1 for $p = 0$ (R^0 is reduced to a point and the measure of the set consisting of this point only is 1). Unless otherwise stated, measurability and integrability on $\mathfrak{R}$ will always be with respect to the above measure. $\mathfrak{A}$ will be identified with the set of all measurable functions on $\mathfrak{R}$ with values in $R \cup \{+\infty\}$ and vanishing outside of a compact (of $\mathfrak{R}$). $\mathfrak{a}$ will be identified with the set of classes of such functions. $\mathfrak{A}_{p+1}$ and $\mathfrak{a}_{p+1}$ will be canonically identified with subsets of $\mathfrak{A}$ and $\mathfrak{a}$ respectively. The addition and the multiplication by an element of R_+^* is defined in $\mathfrak{A}$ and in $\mathfrak{a}$. If $\tilde{A} \in \mathfrak{A}$ and $\tilde{A}$ does not take the value $+\infty$ the product of $\tilde{A}$ by any real number is defined, the product of the class $A \in \mathfrak{a}$ of $\tilde{A}$ by any real number is then also defined. If $\tilde{A}^1, \tilde{A}^2 \in \mathfrak{A}$ and, for all $\xi \in \mathfrak{R}$, either $\tilde{A}^1(\xi) = \tilde{A}^2(\xi) = +\infty$ or $\tilde{A}^1(\xi) - \tilde{A}^2(\xi) \in R_+ \cup \{+\infty\}$ we write $\tilde{A}^1 \geq \tilde{A}^2$, we also write $A^1 \geq A^2$ if $A^1, A^2 \in \mathfrak{a}$ are the classes of $\tilde{A}^1$ and $\tilde{A}^2$ respectively. In what follows, if $\tilde{A} \in \mathfrak{A}$

[4] See for instance N. Bourbaki, *Topologie Générale, Fascicule de Résultats* (Hermann & Cie, Paris, 1953).

has been introduced, we will usually, and without further comment, call its class A. Similarly, if $A \in \mathfrak{A}$ has been introduced, we will note $\tilde{A}$ any element in the class A. If $A \in \mathfrak{A}$ is integrable, its integral will be noted $\int \tilde{A}(\xi)d\xi$.

Let $X = (x_i)_{1\leq i\leq n}$ be a sequence of points in R^ν, $n \in N^*$, and let $\tilde{A}_{p+1} \in \mathfrak{A}_{p+1}$, $p \in N^*$. We define $\tilde{A}_{p+1}[X] = 0$ for $n \leq p$

$$\tilde{A}_{p+1}[X] = \sum \tilde{A}_{p+1}(x_{i_1} - x_{i_0}, \cdots, x_{i_p} - x_{i_0}) \quad \text{for} \quad n > p, \tag{1.2}$$

where the summation extends over the $n!/(n-p-1)!$ sequences $(i_0, i_1, \cdots, i_p)$ of $p+1$ different integers i, with $1 \leq i \leq n$. If $\tilde{A} = (\tilde{A}_{p+1})_{p\in N} \in \mathfrak{A}$ we write also

$$\tilde{A}[X] = n\tilde{A}_1 + \sum_{p\in N^*} \tilde{A}_{p+1}[X]. \tag{1.3}$$

Let now Λ be a measurable subset of finite measure V of R^ν, $\mathbf{A} = (A^\sigma)_{1\leq\sigma\leq q}$ a sequence of elements of $\mathfrak{A}$, $\mathbf{J} = (J^\sigma)_{1\leq\sigma\leq q}$ a sequence of open intervals of R, $q \in N$. The points $X = (x_1, \cdots, x_n)$ of Λ^n, $n \in N^*$, satisfying the conditions $n^{-1}\tilde{A}^\sigma[X] \in J^\sigma$ for $\sigma = 1, \cdots, q$ form a set of measure $n!\mathcal{U}(\Lambda, n; \mathbf{A}, \mathbf{J}) \leq V^n$. $\mathcal{U}(\Lambda, n; \mathbf{A}, \mathbf{J})$ is independent of the choice of the $\tilde{A}^\sigma$ in the classes A^σ and invariant under translations of Λ. Furthermore, if $\Lambda_1 \subset \Lambda_2$,

$$\mathcal{U}(\Lambda_1, n; \mathbf{A}, \mathbf{J}) \leq \mathcal{U}(\Lambda_2, n; \mathbf{A}, \mathbf{J}). \tag{1.4}$$

Let $A^\sigma = (A^\sigma_{p+1})_{p\in N}$ for $\sigma = 1, \cdots, q$. There exists a compact $M \subset R^\nu$ such that, for each $p \in N^*$, $\sigma = 1, \cdots, q$, A^σ_{p+1} reduces to the class of the zero function in the complement of M^ν. We may choose M to be symmetric ($M = -M$) and convex. Defining then Λ' as the subset of Λ formed by the points x such that $x + \frac{1}{2}M \subset \Lambda$, we write

$$\mathcal{U}'(\Lambda, n; \mathbf{A}, \mathbf{J}) = \mathcal{U}(\Lambda', n; \mathbf{A}, \mathbf{J}). \tag{1.5}$$

If Λ_1 and Λ_2 are disjoint we have

$$\mathcal{U}'(\Lambda_1 \cup \Lambda_2, n_1 + n_2; \mathbf{A}, \mathbf{J}) \geq \mathcal{U}'(\Lambda_1, n_1; \mathbf{A}, \mathbf{J})\mathcal{U}'(\Lambda_2, n_2; \mathbf{A}, \mathbf{J}). \tag{1.6}$$

It will be convenient in what follows to choose for M a cube

$$M = \{x: -\kappa \leq x^i \leq \kappa \quad \text{for} \quad i = 1, \cdots, \nu\} \tag{1.7}$$

with $\kappa \in R^*_+$.

2. LIMIT OF AN INFINITE VOLUME

We define sets $\Lambda^\lambda(m) \subset R^\nu$ by

$$\Lambda^\lambda(m) = \{x: 0 \leq x^i < m^i\lambda \quad \text{for} \quad i = 1, 2, \cdots, \nu\}, \tag{2.1}$$

where $\lambda \in R^*_+$, $m = (m^i)_{1\leq i\leq\nu}$ and $m^i \in N^*$ for $i = 1, 2, \cdots, \nu$. Let also $K^\lambda = \Lambda^\lambda(1, 1, \cdots, 1)$. If $n \in N^*$ and $l > \kappa$ we have then

$$\mathcal{U}'(K^l, n; \mathbf{A}, \mathbf{J}) = \mathcal{U}(K^{l-\kappa}, n; \mathbf{A}, \mathbf{J}). \tag{2.2}$$

Let $l(n)$ be the lower bound of the numbers $l > \kappa$ such that $\mathcal{U}(K^{l-\kappa}, n; \mathbf{A}, \mathbf{J}) > 0$. If $\lambda > l(n)$ the function F defined on $(N^*)^\nu$ by

$$F(m) = \log \mathcal{U}'\Big(\Lambda^\lambda(m), n\prod_{i=1}^{\nu} m^i, \mathbf{A}, \mathbf{J}\Big)$$

satisfies the conditions of Lemma A1 (see Appendix) because of (1.6) and we may write

$$n^{-1}\lim\Big(\prod_{i=1}^{\nu} m^i\Big)^{-1} \log \mathcal{U}'\Big(\Lambda^\lambda(m), n\prod_{i=1}^{\nu} m^i; \mathbf{A}, \mathbf{J}\Big) = t^\lambda_n(A, J) < 1 + \log\lambda^\nu/n. \tag{2.3}$$

It follows from (1.4) that t^λ_n is an increasing[5] function of λ. Furthermore if $l(n) < \lambda' < \lambda''$, $\Lambda^{\lambda'+\lambda''}(m)$ contains $\Lambda^{\lambda''}(m)$ and $2^\nu - 1$ mutually disjoint translates of $\Lambda^{\lambda'}(m)$, which are disjoint from $\Lambda^{\lambda''}(m)$. By repeated application of (1.6) and (1.4) this fact yields

$$t^{\frac{1}{2}(\lambda'+\lambda'')}_n > (1 - 2^{-\nu})t^{\lambda'}_n + 2^{-\nu}t^{\lambda''}_n. \tag{2.4}$$

According to Lemma A2 (see Appendix), the above two properties imply that t^λ_n is a continuous function of λ for $\lambda > l(n)$.

Definition 1: If $a = (a^i)_{1\leq i\leq\nu}$, $a^i \in R^*_+$ for $i = 1, \cdots, \nu$, we define a set $\Lambda(a) \subset R^\nu$ by

$$\Lambda(a) = \{x: 0 \leq x^i < a^i \quad \text{for} \quad i = 1, \cdots, \nu\} \tag{2.5}$$

and call $V(a) = \prod_{i=1}^{\nu} a^i$ its measure.

Let $(a_i)_{i\in N}$ be a sequence of elements of $(R^*_+)^\nu$ such that

$$\lim_{i\to\infty}(\min_{1\leq i\leq\nu} a^i_i) = +\infty.$$

Let also $(k_i)_{i\in N}$ be a sequence of elements of N^* such that

$$\lim_{i\to\infty} n_i^{-1}\Lambda(a_i) = \lambda^\nu \in R^*_+.$$

We show that if $\lambda > l(n)$,

$$\lim_{i\to\infty} n^{-1}k_i^{-1} \log \mathcal{U}'(\Lambda(a_i), nk_i; \mathbf{A}, \mathbf{J}) = t^\lambda_n. \tag{2.6}$$

Let $l(n) < \lambda' < \lambda < \lambda''$. We write[6]

$$m_i'^2 = E(a_i^2/\lambda'), \cdots, m_i'^\nu = E(a_i^\nu/\lambda')$$

[5] We call a real function f of a real variable increasing if $\lambda' < \lambda''$ implies $f(\lambda') \leq f(\lambda'')$ whenever $f(\lambda')$ and $f(\lambda'')$ are defined.

[6] We note $E(x)$ the integer part of $x \in R$: $E(x) \in N$ and $0 \leq x - E(x) < 1$.

and $M_i' = \prod_{i=2}^{\nu} m_i'^i$. If $k_i = m_i'^1 M_i' + r_i'$, $m_i'^1 \in N$, $0 \leq r_i' < M_i'$ we have

$$\lim_{j\to\infty} \frac{m_i'^1\lambda'}{a_i^1} = \lim_{j\to\infty} \frac{k_i}{V(a_i)} (\lambda')^\nu = \left(\frac{\lambda'}{\lambda}\right)^\nu < 1; \quad (2.7)$$

hence for j big enough, $m_i'^1\lambda' < a_i^1 - \lambda$. The set $\Lambda(a_i)$ contains then $\Lambda^{\lambda'}(m_i')$ and r_i' mutually disjoint translates of K^λ disjoint from $\Lambda^{\lambda'}(m_i')$, and we have

$$\mathfrak{V}'(\Lambda(a_i), nk_i; \mathbf{A}, \mathbf{J}) \geq \mathfrak{V}'\left(\Lambda^{\lambda'}(m_i'), n\prod_{i=1}^{\nu} m_i'^i; \mathbf{A}, \mathbf{J}\right) \times [\mathfrak{V}'(K^\lambda, n; \mathbf{A}, \mathbf{J})]^{r_i'}. \quad (2.8)$$

When $j \to \infty$, this gives

$$\liminf_{j\to\infty} n^{-1}k_i^{-1} \log \mathfrak{V}'(\Lambda(a_i), nk_i; \mathbf{A}, \mathbf{J}) \geq t_n^{\lambda'}. \quad (2.9)$$

Similarly we write $m_i''^2 = E(a_i^2/\lambda'') + 1, \cdots, m_i''^\nu = E(a_i^\nu/\lambda'') + 1$ and $M_i'' = \prod_{i=2}^{\nu} m_i''^i$. If $k_i = m_i''^1 M_i'' - r_i''$, $m_i''^1 \in N^*$, $0 \leq r_i'' < M_i''$, we have

$$\lim_{i\to\infty} \frac{m_i''^1\lambda''}{a_i^1} = \lim_{i\to\infty} \frac{k_i}{V(a_i)} (\lambda'')^\nu = \left(\frac{\lambda''}{\lambda}\right)^\nu > 1, \quad (2.10)$$

hence for j big enough, $m_i''^1\lambda'' > a_i^1 + \lambda$. The set $\Lambda^{\lambda''}(m_i'')$ contains then $\Lambda(b_i)$ and r_i'' mutually disjoint translates of K^λ disjoint from $\Lambda(b_i)$ and we have

$$\mathfrak{V}'\left(\Lambda^{\lambda''}(m_i''), n\prod_{i=1}^{\nu} m_i''^i; \mathbf{A}, \mathbf{J}\right) \geq \mathfrak{V}'(\Lambda(a_i), nk_i; \mathbf{A}, \mathbf{J})[\mathfrak{V}'(K^\lambda, n; \mathbf{A}, \mathbf{J})]^{r_i''}. \quad (2.11)$$

When $j \to \infty$ this gives

$$t_n^{\lambda''} \geq \limsup_{j\to\infty} n^{-1}k_i^{-1} \log \mathfrak{V}'(\Lambda(a_i), nk_i; \mathbf{A}, \mathbf{J}). \quad (2.12)$$

Since λ' and λ'' may be chosen arbitrarily close to λ, and t_n^λ is continuous in λ, (2.6) follows from (2.9) and (2.12).

Let $\mathbf{J}' = (J'^\sigma)_{1\leq\sigma\leq q}$ be a sequence of open intervals of R such that the closure of J'^σ belongs to J^σ for $\sigma = 1, \cdots, q$. Since $\mathfrak{V}(K^{\lambda-\kappa}, n; \mathbf{A}, \mathbf{J}) > 0$, if $\lambda > l(n)$, $\mathbf{J}'$ may be chosen such that $\mathfrak{V}(K^{\lambda-\kappa}, n; \mathbf{A}, \mathbf{J}') > 0$. Let $r \in N^*$, $0 < r \leq n$. The cube K^l contains $\Lambda^\lambda(m)$ and r mutually disjoint translates $K_1, \cdots, K_r$ of K^λ disjoint from $\Lambda^\lambda(m)$ provided

$$l \geq (n + \max_{1\leq i\leq\nu} m^i)\lambda.$$

Let $M = \prod_{i=1}^{\nu} m^i$. If $X = (x_1, \cdots, x_{nM}) \in [(\Lambda^\lambda(m))']^{nM}$ and $x_{nM+1} \in (K_1)', \cdots, x_{nM+r} \in (K_r)'$, we write $X' = (x_1, \cdots, x_{nM+r}) \in [(K^l)']^{nM+r}$. We have $A^\sigma[X'] = A^\sigma[X]$ for $\sigma = 1, \cdots, q$, hence for M big enough,

$$\mathfrak{V}'(K^l, nM + r; \mathbf{A}, \mathbf{J}) \geq \mathfrak{V}'(K^\lambda(m), nM; \mathbf{A}, \mathbf{J}')(\lambda - \mu)^{\nu r}. \quad (2.13)$$

There exists thus $l \in R_+^*$ and $M \in N$ such that for $r = 0, 1, \cdots, n$,

$$\mathfrak{V}'(K^l, nM + r; \mathbf{A}, \mathbf{J}) > 0. \quad (2.14)$$

We write $b_i = (a_i^1 + \kappa, a_i^2 + \kappa, \cdots, a_i^\nu + \kappa)$, $c = (l, l, \cdots, l) \in (R_+^*)^\nu$. Let $(n_i)_{i\in N}$ be a sequence of elements of N^* such that

$$\lim_{i\to\infty} n_i^{-1} V(a_i) = n^{-1}\lambda^\nu.$$

We write $n_i = nk_i + r_i$, $k_i \in N$, $0 \leq r_i < n$. For j big enough we have $n_i > nM$ and $a_i > l + \kappa$, then

$$\mathfrak{V}(\Lambda(a_i), n_i; \mathbf{A}, \mathbf{J})\mathfrak{V}'(K^l, n(M + 1) - r_i; \mathbf{A}, \mathbf{J}) \leq \mathfrak{V}'(\Lambda(b_i + c), n(k_i + M + 1); \mathbf{A}, \mathbf{J}) \quad (2.15)$$

$$\mathfrak{V}'(\Lambda(b_i - c), n(k_i - M); \mathbf{A}, \mathbf{J})\mathfrak{V}'(K^l, nM + r_i; \mathbf{A}, \mathbf{J}) \leq \mathfrak{V}(\Lambda(a_i), n_i; \mathbf{A}, \mathbf{J}). \quad (2.16)$$

From (2.15), (2.16), and (2.6) we obtain

$$\lim_{i\to\infty} n_i^{-1} \log \mathfrak{V}(\Lambda(a_i), n_i; \mathbf{A}, \mathbf{J}) = t_n^\lambda. \quad (2.17)$$

Let $n_1, n_2 \in N^*$ and $\lambda_1, \lambda_2 \in R_+^*$. If $n_1^{-1}\lambda_1^\nu = n_2^{-1}\lambda_2^\nu = v$ and $\lambda_1 > l(n_1)$, $\lambda_2 > l(n_2)$, it follows from (2.17) that $t_{n_1}^{\lambda_1}(\mathbf{A}, \mathbf{J}) = t_{n_2}^{\lambda_2}(\mathbf{A}, \mathbf{J}) = t(v, \mathbf{A}, \mathbf{J})$. Considered as a function of v, t is defined only if we assume, as we did, that $\mathfrak{V}'(K^\lambda, n; A, J) > 0$ for some $n \in N^*$ and some $\lambda \in R_+^*$. In this case it is defined for $v \in R_+^*$, $v > v_0$, where $v_0 = \inf_{n\in N^*} n^{-1}[l(n)]^\nu \in R_+$.

Proposition 1: Given sequences $A = (A^\sigma)_{1\leq\sigma\leq q}$ *and* $\mathbf{J} = (J^\sigma)_{1\leq\sigma\leq q}$ *the following two possibilities exist:*

(1) *For all* $a \in (R_+^*)^\nu$ *and* $n \in N^*$,

$$\mathfrak{V}(\Lambda(a), n; \mathbf{A}, \mathbf{J}) = 0;$$

(2) *there exists* $v_0 \in R_+$ *and a real function* $t(v; \mathbf{A}, \mathbf{J})$ *defined for* $v > v_0$, *satisfying the following requirements*:

For all $a \in (R_+^*)^\nu$ *and* $n \in N^*$ *such that* $n^{-1}V(a) \leq v_0$, $\mathfrak{V}'(\Lambda(a), n; \mathbf{A}, \mathbf{J}) = 0$

For all $a \in (R_+^*)^\nu$ *and* $n \in N^*$ *such that* $\mathfrak{V}'(\Lambda(a), n; \mathbf{A}, \mathbf{J}) > 0$,

$$n^{-1} \log \mathfrak{V}'(\Lambda(a), n; \mathbf{A}, \mathbf{J}) \leq t(n^{-1}V(a); \mathbf{A}, \mathbf{J}). \quad (2.18)$$

If $(a_i)_{i\in N}$ *is a sequence of elements of* $(R_+^*)^\nu$ *such that* $\lim_{i\to\infty} (\min_{1\leq i\leq\nu} a_i^i) = +\infty$ *and* $(n_i)_{i\in N}$ *a sequence of elements of* N^* *such that* $\lim_{i\to\infty} n_i^{-1}V(a_i) = v \in R_+^*$ *and* $v > v_0$,

$$\lim_{i\to\infty} n_i^{-1} \log \mathfrak{V}'(\Lambda(a_i), n_i; \mathbf{A}, \mathbf{J}) = t(v; \mathbf{A}, \mathbf{J})$$
$$\lim_{i\to\infty} n_i^{-1} \log \mathfrak{V}(\Lambda(a_i), n_i; \mathbf{A}, \mathbf{J}) = t(v; \mathbf{A}, \mathbf{J}). \quad (2.19)$$

The function $t(v; \mathbf{A}, \mathbf{J})$ *is continuous, increasing, and*

satisfies the inequality

$$t(v; A, J) \leq 1 + \log v. \tag{2.20}$$

Instead of the sequence $(\Lambda(a_i))_{i\in N}$ one could use a more general sequence $(\Lambda_i)_{i\in N}$ of sets $\Lambda_i \in R^\nu$ with measure V_i such that $\lim_{i\to\infty} n_i^{-1}V_i = v \in R_+^*$, $v > v_0$. Let us only mention that if every Λ_i is convex and if, for all $L \in R_+^*$, Λ_i contains a translate of K^L for j big enough, (2.19) still holds with $\Lambda(a_i)$ replaced by Λ_i.

3. DEFINITION AND PROPERTIES OF THE FUNCTION $s(A, E)$

If $\mathbf{J}_1 = (J_1^\sigma)_{1\leq\sigma\leq q}$, $\mathbf{J}_2 = (J_2^\sigma)_{1\leq\sigma\leq q}$, $q \in N$ are sequences of open intervals of R, $\mathbf{J}_1$, and $\mathbf{J}_2$ may be identified with open sets of R^q. We define then $\mathbf{J}_1 + \mathbf{J}_2$ as the set of all sums of an element of $\mathbf{J}_1$ and an element of $\mathbf{J}_2$, the product λJ, $\lambda \in R$, is defined as the set of all products of an element of $\mathbf{J}$ by λ.

If $a, a_1, a_2 \in (R_+^*)^\nu$ are such that $\Lambda(a)$ is the union of $\Lambda(a_1)$ and of a translate of $\Lambda(a_2)$ disjoint from $\Lambda(a_1)$ and if $n_1, n_2 \in N^*$, we have

$$\mathcal{V}'(\Lambda(a), n_1 + n_2; \mathbf{A}, (n_1\mathbf{J}_1 + n_2\mathbf{J}_2)/(n_1 + n_2)) \geq \mathcal{V}'(\Lambda(a_1), n_1; \mathbf{A}, \mathbf{J}_1)\mathcal{V}'(\Lambda(a_2), n_2; \mathbf{A}, \mathbf{J}_2); \tag{3.1}$$

hence, if $v_1, v_2 \in R_+^*$, Proposition 1 shows that

$$t(\alpha v_1 + (1-\alpha)v_2; \mathbf{A}, \alpha\mathbf{J}_1 + (1-\alpha)\mathbf{J}_2) \geq \alpha t(v_1; \mathbf{A}, \mathbf{J}_1) + (1-\alpha)t(v_2; \mathbf{A}, \mathbf{J}_2), \tag{3.2}$$

provided $t(v_1; \mathbf{A}, \mathbf{J}_1)$ and $t(v_2; \mathbf{A}, \mathbf{J}_2)$ are defined and $0 < \alpha < 1$. If $\mathbf{J}' \subset \mathbf{J}$ and $t(v; \mathbf{A}, \mathbf{J}')$ is defined we have

$$t(v; \mathbf{A}, \mathbf{J}') \leq t(v; \mathbf{A}, \mathbf{J}). \tag{3.3}$$

From Proposition 1 it follows that if $t(v; \mathbf{A}, \mathbf{J})$ is defined and $\mathbf{J} = \bigcup_i \mathbf{J}_i$ is a finite union of sets $\mathbf{J}_i$,

$$t(v; \mathbf{A}, \mathbf{J}) = \max_i t(v; \mathbf{A}, \mathbf{J}_i); \tag{3.4}$$

the maximum being taken over the indices j for which $t(v; \mathbf{A}, \mathbf{J}_i)$ is defined. It follows also that for any $\epsilon \in R_+^*$ one can find $\mathbf{J}'$ with compact closure $\mathbf{J}_\epsilon'$ such that $\mathbf{J}_\epsilon' \subset \mathbf{J}$ and

$$\mathcal{V}'(\Lambda, n; \mathbf{A}, \mathbf{J}') \geq \mathcal{V}'(\Lambda, n; \mathbf{A}, \mathbf{J}) - \epsilon. \tag{3.5}$$

Hence $t(v; \mathbf{A}, \mathbf{J})$ is, if it is defined, the supermum of all defined $t(v; \mathbf{A}, \mathbf{J}')$ for $\mathbf{J}'$ relatively compact in $\mathbf{J}$.

Definition 2. Let $\mathbf{F} = (F^\sigma)_{1\leq\sigma\leq q}$ be a sequence of real numbers (i.e., $F \in R^q$). If $t(v; A, J)$ is defined for all $J \ni F$ and inf $t(v; a, J)$ *exists in R we define*

$$t(v; \mathbf{A}, \mathbf{F}) = \inf_{\mathbf{J}\ni\mathbf{F}} t(v; \mathbf{A}, \mathbf{J}). \tag{3.6}$$

We call $Q(v)$ the subset of R^q on which $t(v; \mathbf{A}, \mathbf{F})$ is defined.

It follows from (3.2) that

$$t(\alpha v_1 + (1-\alpha)v_2; \mathbf{A}, \alpha\mathbf{F}_1 + (1-\alpha)\mathbf{F}_2) \geq \alpha t(v_1; \mathbf{A}, \mathbf{F}_1) + (1-\alpha)t(v_2; \mathbf{A}, \mathbf{F}_2) \tag{3.7}$$

provided $t(v_1; \mathbf{A}, \mathbf{F}_1)$ and $t(v_2; \mathbf{A}_1, \mathbf{F}_2)$ are defined.

If $t(v; \mathbf{A}, \mathbf{J}) = t$ is defined, for any $\epsilon \in R_+^*$ one may choose $\mathbf{J}'$ relatively compact in $\mathbf{J}$ such that $t(v; \mathbf{A}, \mathbf{J}') = t'$ is defined and $t' \geq t - \epsilon$. There exists by (4) a decreasing sequence $(\mathbf{J}_i)_{i\in N}$ of subsets of $\mathbf{J}'$ converging towards a point $\mathbf{F}'$ of the closure of $\mathbf{J}'$ and such that $t(v; \mathbf{A}, \mathbf{J}_i) = t'$ for all j. By (3.3) and (3.6), $t(v; \mathbf{A}, \mathbf{F}')$ is then defined and $\geq t - \epsilon$. This shows that $t(v; \mathbf{A}, \mathbf{J})$ is defined if and only if $\mathbf{J}$ is not disjoint from $Q(v)$. Furthermore, if $t(v; \mathbf{A}, \mathbf{J})$ is defined, for any $\epsilon \in R_+^*$ there exists $\mathbf{F}' \in \mathbf{J} \cap Q(v)$ such that

$$t(v; \mathbf{A}, \mathbf{J}) - \epsilon \leq t(v; \mathbf{A}, \mathbf{F}'); \tag{3.8}$$

hence

$$t(v; \mathbf{A}, \mathbf{J}) \leq \sup_{\mathbf{F}\in\mathbf{J}\cap Q(v)} t(v; \mathbf{A}, \mathbf{F}). \tag{3.9}$$

On the other hand, by (3.6)

$$t(v; \mathbf{A}, \mathbf{J}) \geq \sup_{\mathbf{F}\in\mathbf{J}\cap Q(v)} t(v; \mathbf{A}, \mathbf{F}). \tag{3.10}$$

Proposition 2: The function $t(v; \mathbf{A}, \mathbf{F})$ of v and $\mathbf{F}$ is defined and concave[7] *on a convex subset of $R_+^* \times R^q$. $t(v; \mathbf{A}, \mathbf{J})$ is defined if and only if $\mathbf{J} \cap Q(v) \neq \phi$, and then*

$$t(v; \mathbf{A}, \mathbf{J}) = \sup_{\mathbf{F}\in\mathbf{J}\cap Q(v)} t(v; \mathbf{A}, \mathbf{F}). \tag{3.11}$$

Let again Λ be a measurable subset of finite measure V of R^ν and $\mathbf{I} = (I^\sigma)_{1\leq\sigma\leq q}$ a sequence of open intervals of R, $q \in N$. For each $n \in N^*$ the measure of the subset of Λ^n formed by all X such that $V^{-1}\tilde{A}^\sigma[X] \in I^\sigma$ for $\sigma = 1, \cdots, q$ is $\mathcal{V}(\Lambda, n; \mathbf{A}, V/n\mathbf{I})$. The following series converge

$$\mathcal{U}'(\Lambda; \mathbf{A}, \mathbf{I}) = \sum_{n\in N^*} \mathcal{V}'\left(\Lambda, n; \mathbf{A}, \frac{V}{n}\mathbf{I}\right) < e^V,$$
$$\mathcal{U}(\Lambda; \mathbf{A}, \mathbf{I}) = \sum_{n\in N^*} \mathcal{V}\left(\Lambda, n; \mathbf{A}, \frac{V}{n}\mathbf{I}\right) < e^V. \tag{3.12}$$

Consider now the functions of $d \in R_+^*$ defined by

$$s(d; \mathbf{A}, \mathbf{I}) = dt(d^{-1}; \mathbf{A}, d^{-1}\mathbf{I}) \leq d(1 - \log d) \leq 1, \tag{3.13}$$

[7] Let Q be a convex set (in a real vector space). We call a real function f, defined on Q, concave if for any α such that $0 < \alpha < 1$ and any $\zeta_1, \zeta_2 \in Q$ the following inequality holds $f(\alpha\zeta_1 + (1-\alpha)\zeta_2) \geq \alpha f(\zeta_1) + (1-\alpha) f(\zeta_2)$.

$$s(d; \mathbf{A}, \mathbf{E}) = dt(d^{-1}; \mathbf{A}, d^{-1}\mathbf{E}) \leq d(1 - \log d) \leq 1. \quad (3.14)$$

Let $d_1, d_2 \in R_+^*$, $\mathbf{I}_1, \mathbf{I}_2$ be sequences of open intervals of R and $0 < \alpha < 1$. If we replace in (3.2) α by $[\alpha d_1 + (1-\alpha)d_2]^{-1}\alpha d_1$ and put $v_1 = d_1^{-1}$, $v_2 = d_2^{-1}$, $\mathbf{J}_1 = d_1^{-1}\mathbf{I}_1$, $\mathbf{J}_2 = d_2^{-1}\mathbf{I}_2$ we obtain

$$s(\alpha d_1 + (1-\alpha)d_2; \mathbf{A}, \alpha\mathbf{I}_1 + (1-\alpha)\mathbf{I}_2) \geq \alpha s(d_1; \mathbf{A}, \mathbf{I}_1) + (1-\alpha)s(d_2; \mathbf{A}, \mathbf{I}_2) \quad (3.15)$$

provided $s(d_1; \mathbf{A}, \mathbf{I}_1)$ and $s(d_2; \mathbf{A}, \mathbf{I}_2)$ are defined. Similarly, using (3.7) we obtain

$$s(\alpha d_1 + (1-\alpha)d_2; \mathbf{A}, \alpha\mathbf{E}_1 + (1-\alpha)\mathbf{E}_2) \geq \alpha s(d_1; \mathbf{A}, \mathbf{E}_1) + (1-\alpha)s(d_2; \mathbf{A}, \mathbf{E}_2), \quad (3.16)$$

provided $s(d_1; \mathbf{A}, \mathbf{E}_1)$ and $s(d_2; \mathbf{A}, \mathbf{E}_2)$ are defined. In particular $s(d; \mathbf{A}, \mathbf{I})$ is a concave function of d on its interval of definition $I \subset R_+^*$. It follows from Proposition 2 that I either is empty or has a nonempty interior.

By Proposition 1, if I is empty $\mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I}) = 0$ for any $a \in (R_+^*)^\nu$. If I is not empty we define

$$s(\mathbf{A}, \mathbf{I}) = \sup_{d \in I} s(d; \mathbf{A}, \mathbf{I}). \quad (3.17)$$

To any $V_0 \in R_+^*$, $s \in R$, we can find two intervals I' and I'' of R such that $I = I' \cup I''$, I' is bounded and, for any $V \geq V_0$,

$$\sum_{n \in VI''} \frac{V^n}{n!} \leq \exp(Vs). \quad (3.18)$$

Taking $s = s(\mathbf{A}, \mathbf{I})$ we have then

$$V(a)^{-1} \log \mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I}) = V(a)^{-1} \log \sum_{n \in VI} \mathfrak{V}'\left(\Lambda(a), n; \mathbf{A}, \frac{V}{n}\mathbf{I}\right) \leq V(a)^{-1} \log \sum_{n \in VI'} \mathfrak{V}'\left(\Lambda(a), n; \mathbf{A}, \frac{V}{n}\mathbf{I}\right) + \exp[V(a)s(\mathbf{A}, \mathbf{I})] \quad (3.19)$$

$$V(a)^{-1} \log \mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I}) \geq V(a)^{-1} \log \left[\max_{n \in VI} \mathfrak{V}'\left(\Lambda, n; \mathbf{A}, \frac{V}{n}\mathbf{I}\right)\right] \quad (3.20)$$

so that, given $\epsilon \in R_+^*$, one can find $l \in R_+^*$ such that

$$s(\mathbf{A}, \mathbf{I}) + \epsilon > V(a)^{-1} \log \mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I}) > s(\mathbf{A}, \mathbf{I}) - \epsilon \quad (3.21)$$

provided $\min_{1 \leq i \leq \nu} a^i > l$.

If $s(d; \mathbf{A}, \mathbf{E})$ is defined for some $d \in R_+^*$ and $\mathbf{E} \in R^q$ we define

$$\bar{s}(\mathbf{A}, \mathbf{E}) = \sup s(d; \mathbf{A}, \mathbf{E}), \quad (3.22)$$

where the supremum is taken over d in the interval of definition of $s(d; \mathbf{A}, \mathbf{E})$. Let $\tilde{P}$ be the convex subset of R^q where the concave function $\bar{s}(\mathbf{A}, \mathbf{E})$ of $\mathbf{E}$ is defined. It follows from Proposition 2 that $s(\mathbf{A}, \mathbf{I})$ is defined if and only if $\mathbf{I}$ and $\tilde{P}$ are not disjoint and in this case

$$s(\mathbf{A}, \mathbf{I}) = \sup_{\mathbf{E} \in \mathbf{I} \cap \tilde{P}} \bar{s}(\mathbf{A}, \mathbf{E}). \quad (3.23)$$

Conversely if $s(\mathbf{A}, \mathbf{I})$ is defined for every $\mathbf{I} \ni \mathbf{E}$, and $\inf s(\mathbf{A}, \mathbf{I})$ exists in R, we define

$$s(\mathbf{A}, \mathbf{E}) = \inf_{\mathbf{I} \ni \mathbf{E}} s(\mathbf{A}, \mathbf{I}). \quad (3.24)$$

Let P be the subset of R^q where $s(\mathbf{A}, \mathbf{E})$ is defined. It is clear that $P \supset \tilde{P}$ and $s(\mathbf{A}, \mathbf{E}) \geq \bar{s}(\mathbf{A}, \mathbf{E})$. Furthermore $s(\mathbf{A}, \mathbf{E})$ is concave on the convex set P and, for every $s_0 \in R$, the set $\{E : s(A, E) \geq s_0\}$ is closed in R^q [in particular, $s(\mathbf{A}, \mathbf{E})$ is upper semi-continuous on P]. It follows also from (3.23) and (3.24) that $s(\mathbf{A}, \mathbf{I})$ is defined if and only if $\mathbf{I}$ and P are not disjoint and in this case

$$s(\mathbf{A}, \mathbf{I}) = \sup_{\mathbf{E} \in \mathbf{I} \cap P} s(\mathbf{A}, \mathbf{E}). \quad (3.25)$$

Notice finally that if $a \in (R_+^*)^\nu$ and $b = (a^1 + \kappa, \cdots, a^\nu + \kappa)$ we have

$$\mathfrak{U}(\Lambda(a); \mathbf{A}, \mathbf{I}) = \mathfrak{U}'\left(\Lambda(b); \mathbf{A}, \frac{V(a)}{V(b)}\mathbf{I}\right).$$

If $s(\mathbf{A}, \mathbf{I})$ is defined, for any $\epsilon \in R_+^*$ one can find $\mathbf{I}'$ such that the closure of $\mathbf{I}$ is contained in $\mathbf{I}'$ and $s(\mathbf{A}, \mathbf{I}') - s(\mathbf{A}, \mathbf{I}) < \epsilon$. Using (3.21) we have thus for $\min_{1 \leq i \leq \nu} a^i$ sufficiently large

$$\mathfrak{U}'(\Lambda(b); \mathbf{A}, \mathbf{I}') > \mathfrak{U}(\Lambda(a); \mathbf{A}, \mathbf{I}) > \mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I}) \quad (3.26)$$

$$s(\mathbf{A}, \mathbf{I}) + 2\epsilon > V(a)^{-1} \log \mathfrak{U}(\Lambda(a); \mathbf{A}, \mathbf{I}) > s(\mathbf{A}, \mathbf{I}) - \epsilon. \quad (3.27)$$

Theorem 1: Given sequences $\mathbf{A} = (A^\sigma)_{1 \leq \sigma \leq q}$ *and* $\mathbf{I} = (I^\sigma)_{1 \leq \sigma \leq q}$ *there exists a real function* $s(\mathbf{A}, \mathbf{E})$ *defined when* $\mathbf{E}$ *belongs to a convex set* P *of* R^q *and satisfying the following requirements:*

(1) *If* $\mathbf{I} \cap P = \phi$, $t(v; \mathbf{A}, v\mathbf{I})$ *is defined for no* $v \in R_+^*$ *and* $\mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I}) = 0$ *for all* $a \in (R_+^*)^\nu$.

(2) *If* $\mathbf{I} \cap P \neq \phi$ *the limits when*

$$\min_{1 \leq i \leq \nu} a^i$$

tends to infinity of $V(a)^{-1} \log \mathfrak{U}(\Lambda(a); \mathbf{A}, \mathbf{I})$ *and* $V(a)^{-1} \log \mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I})$ *exist in* R *and coincide, defining a number*

$$s(\mathbf{A}, \mathbf{I}) = \sup_{\mathbf{E} \in \mathbf{I} \cap P} s(\mathbf{A}, \mathbf{E}). \quad (3.28)$$

In this case $t(v; \mathbf{A}, v\mathbf{I})$ *is defined for some* v *and*

$$s(\mathbf{A}, \mathbf{I}) = \sup_v v^{-1} t(v; \mathbf{A}, v\mathbf{I}). \tag{3.29}$$

$s(\mathbf{A}, \mathbf{E})$ *is defined if and only if* $s(\mathbf{A}, \mathbf{I})$ *is defined for all* $\mathbf{I} \ni \mathbf{E}$ *and* $\inf s(\mathbf{A}, \mathbf{I})$ *exists in* R, *then*

$$s(\mathbf{A}, \mathbf{E}) = \inf_{\mathbf{I} \ni \mathbf{E}} s(\mathbf{A}, \mathbf{I}) \tag{3.30}$$

$s(\mathbf{A}, \mathbf{E})$ *is concave, bounded by* 1 *on* P, *and for every* $s_0 \in R$ *the set* $\{\mathbf{E} : s(\mathbf{A}, \mathbf{E}) \geq s_0\}$ *is closed in* R^q.

It may be noticed that if the set P is not empty it contains the origin of R^q and $s(\mathbf{A}, 0) \geq 0$. For the purpose of later reference we note the following result

Corollary. Let $A = (A^1, \cdots, A^q)$, $\mathbf{A}' = (A^1, \cdots, A^q, A^{q+1})$ *and* $\mathbf{I} = (I^1, \cdots, I^q)$. *We assume that* $\bar{A}^{q+1}$ *may take the value* $+\infty$ *only at points of* $\mathfrak{R}$ *for which some* $\bar{A}^\sigma$, $1 \leq \sigma \leq q$, *takes the value* $+\infty$. *Then* $s(\mathbf{A}', \mathbf{I} \times R)$ *is defined if and only if* $s(\mathbf{A}, \mathbf{I})$ *is defined, and in the latter case*

$$s(\mathbf{A}', \mathbf{I} \times R) = s(\mathbf{A}, \mathbf{I}). \tag{3.31}$$

4. CORRELATION DATA

Definition 3: We call correlation data any couple $(\mathcal{P}, \rho)$ *of a part* $\mathcal{P}$ *of* $\mathfrak{A}$ *and of a function* ρ *from* $\mathcal{P}$ *to* R. *We say that the correlation data* $(\mathcal{P}, \rho)$ *are compatible if the infimum of* $s(\mathbf{A}, \mathbf{E})$, *where* $\mathbf{A}$ *is a finite sequence of elements of* $\mathcal{P}$ *and* $\mathbf{E} = \rho(\mathbf{A})$, *exists in* R. *This infimum will then be noted* $s(\mathcal{P}, \rho)$.

The couples $(\mathbf{A}, \mathbf{E})$ considered in Sec. 3 are in an obvious sense equivalent to correlation data $(\mathcal{P}, \rho)$ where $\mathcal{P}$ is a finite set. We note the following easily proved result.

Proposition 3: Let the correlation data $(\mathcal{P}, \rho)$ *be compatible. If* $A^1, A^2, A^1 + A^2 \in \mathcal{P}$, *then* $\rho(A^1 + A^2) = \rho(A^1) + \rho(A^2)$. *If* $\alpha \in R$ *and* A, $\alpha A \in \mathcal{P}$, *then* $\rho(\alpha A) = \alpha\rho(A)$. *If* $A^1, A^2 \in \mathcal{P}$, $\alpha \in R_+^*$, *and* $A^1 \geq \alpha A^2$, *then* $\rho(A^1) \geq \alpha\rho(A^2)$.

If $\mathbf{A}_{(1)} = (A^\sigma_{(1)})_{1 \leq \sigma \leq q}$, $\mathbf{A}_{(2)} = (A^\sigma_{(2)})_{1 \leq \sigma \leq q}$ *and if* $s((A_{(1)}, A_{(2)}), (E_{(1)}, E_{(2)}))$ *is defined, then* $s(A_{(1)} + A_{(2)}, E_{(1)} + E_{(2)})$ *is defined and*

$$s(A_{(1)} + A_{(2)}, E_{(1)} + E_{(2)}) \geq s((A_{(1)}, A_{(2)}), (E_{(1)}, E_{(2)})) \tag{4.1}$$

Definition 4: We will call $\mathcal{C}^K$ *(resp.* $\mathfrak{B}^K$*) the space of real continuous functions (resp. of classes of real bounded measurable functions) vanishing outside of a compact* $K \subset \mathfrak{R}$, *and* $\mathcal{C}$ *(resp.* $\mathfrak{B}$*) the union over* K *of the spaces* $\mathcal{C}^K$ *(resp.* $\mathfrak{B}^K$*). We call* $\mathcal{K}$ *the space of classes of real locally integrable functions on* $\mathfrak{R}$.

We will also write $\mathcal{C}_{p+1} = \mathcal{C} \cap \mathfrak{A}_{p+1}$ (resp. $\mathfrak{B}_{p+1} = \mathfrak{B} \cap \mathfrak{A}_{p+1}$). Clearly then $\mathcal{C}$ (resp. $\mathfrak{B}$) is a real vector space, direct sum of the $\mathcal{C}_{p+1}$ (resp. $\mathfrak{B}_{p+1}$). One may write $K = (K_{p+1})_{p \in N}$, then K is a compact in $\mathfrak{R}$ if and only if, for each $p \in N$, K_{p+1} is a compact in $R^{p\nu}$ and only a finite number of terms of the sequence are not empty. $C = (C_{p+1})_{p \in N} \in \mathcal{C}^K$ means that, for each $p \in N$, C_{p+1} is a real continuous function vanishing outside of K_{p+1}. $B = (B_{p+1})_{p \in N} \in \mathfrak{B}^K$ means that, for each $p \in N$, B_{p+1} is a class of real measurable function vanishing outside of K_{p+1}. $\mathcal{C}^K$ and $\mathfrak{B}^K$ will be considered as Banach spaces for the norms

$$||C|| = \max_{\xi \in \mathfrak{R}} |C(\xi)|, \quad ||B|| = \operatorname*{ess.\,sup.}_{\xi \in \mathfrak{R}} |\tilde{B}(\xi)| \tag{4.2}$$

respectively. $\mathcal{C}^K$ is a subspace of $\mathfrak{B}^K$. One has the inclusions $\mathfrak{A} \supset \mathfrak{B} \supset \mathcal{C}$.

Let the data $(\mathcal{C}, \rho)$ be compatible. ρ is linear from $\mathcal{C}$ to R and $\rho(C) \geq 0$ if $C \geq 0$. From this results that the restriction of ρ to every $\mathcal{C}^K$ is continuous: ρ is a positive measure. Similarly, if the data $(\mathfrak{B}, \rho)$ are compatible, the restriction of ρ to every $\mathfrak{B}^K$ is continuous. We will now obtain more information about ρ.

Let χ be a real continuous function ≥ 0 with compact support, equal to 1 on a set $L \subset R^\nu$ which is symmetric ($L = -L$), convex and compact. Let $\tilde{\omega}$ be a measurable function, $0 \leq \tilde{\omega} \leq 1$, vanishing outside of a measurable set $W \subset R^{p\nu}$, $p \in N^*$, of measure w. We call a sequence $(x_0, x_1, \cdots, x_p)$ of elements of R^ν an "ω sequence" if $\tilde{\omega}(x_1 - x_0, \cdots, x_p - x_0) > 0$ and assume that, whenever $(x_0, x_1, \cdots, x_p)$ is an ω sequence, all the differences $x_i - x_i$, for $0 \leq i < j \leq p$, belong to $\frac{1}{2}L$.

Let now $X = (x_i)_{1 \leq i \leq n}$, $n \in N^*$, be a sequence of elements of a measurable set $\Lambda \subset R^\nu$ of measure V. We call $n_l[X]$, $l \geq p$, the number of elements x_i of X satisfying the following two conditions:

(1) There exists an ω-sequence containing x_i formed with different elements of X.

(2) The set $x_i + L \subset R^\nu$ contains exactly l elements of X different from x_i. x_i belongs thus to at most $(p+1)[l!/(l-p)!]$ ω-sequences and therefore

$$\tilde{\omega}[X] \leq \sum_{l=p}^{\infty} \frac{l!}{(l-p)!} n_l[X]. \tag{4.3}$$

If we write, for $p_1 \geq p$

$$\chi_{p_1+1}(\xi_1, \xi_2, \cdots, \xi_{p_1}) = \chi(\xi_1)\chi(\xi_2) \cdots \chi(\xi_{p_1}), \tag{4.4}$$

we have also

$$\chi_{p_1+1}[X] \geq \sum_{l=p_1}^{\infty} \frac{l!}{(l-p_1)!} n_l[X]. \tag{4.5}$$

Let now $p+2 \leq p_1 < p_2$, we have

$$\tilde{\omega}[X] \leq \sum_{l=p}^{p_2} \frac{l!}{(l-p)!} n_l[X] + \sum_{l=p_2+1}^{\infty} \frac{(l-p_1)!}{(l-p)!} \frac{l!}{(l-p_1)!} n_l[X], \quad (4.6)$$

$$\frac{l!}{(l-p_1)!} n_l[X] < \chi_{p_1+1}[X] \quad \text{for} \quad l \geq p_1, \quad (4.7)$$

and the series

$$\sum_{l=p_1}^{\infty} \frac{(l-p_1)!}{(l-p)!} = \sum_{l=0}^{\infty} \frac{l!}{(l+p_1-p)!} = \frac{1}{p_1-p-1} \cdot \frac{1}{(p_1-p-1)!} \quad (4.8)$$

converges. To any $\epsilon \in R_+^*$ we may therefore choose p_2 such that

$$\sum_{l=p_2+1}^{\infty} \frac{(l-p_1)!}{(l-p)!} < \epsilon; \quad (4.9)$$

hence

$$\tilde{\omega}[X] < \frac{p_2!}{(p_2-p)!} \sum_{l=p}^{p_2} n_l[X] + \epsilon \chi_{p_1+1}[X]. \quad (4.10)$$

Let

$$n_+[X] = \sum_{l=p}^{p_2} n_l[X]. \quad (4.11)$$

If X is any sequence of n points of Λ for which $n_+[X] \geq n_+$, $n_+ \in R_+$, there exist at least $E(n_+/(p_2+1))$ ω sequences formed with disjoint $(p+1)$-tuples of elements of X. If $n!\mathcal{U}(\Lambda, n, n_+)$ is the measure of the subset of Λ^n formed by the sequences X for which $n_+[X] \geq n_+$ we have therefore

$$n!\,\mathcal{U}(\Lambda, n, n_+) \leq \frac{n!\, w^{E(n_+/(p_2+1))} V^{n-pE(n_+/(p_2+1))}}{[n-(p+1)E(n_+/(p_2+1))]!\,[E(n_+/(p_2+1))]!}. \quad (4.12)$$

Let J_1 be the interval $(-\mu, +\mu)$ of R, where $\mu > 0$, and J_2 the interval $(\alpha(p_2+1)p_2!/(p_2-p)! + \epsilon\mu, +\infty)$, where $0 < \alpha < 1/(p_2+1)$. We have

$$\mathcal{U}(\Lambda, n; (\chi_{p_1+1}, \omega), (I_1, I_2)) \leq \mathcal{U}(\Lambda, n, \alpha(p_2+1)n); \quad (4.13)$$

hence, if $t(v; (\chi_{p_1+1}, \omega), (I_1, I_2))$ is defined,

$$t(v; (\chi_{p_1+1}, \omega), (I_1, I_2)) \leq F(v; w, \alpha) = \alpha \log w/\alpha + (1-p\alpha)(1+\log v) - [1-(p+1)\alpha] \log [1-(p+1)\alpha]. \quad (4.14)$$

Let now the correlation data $(\mathcal{P}, \rho)$ be compatible, where $\mathcal{P}$ is either $\mathcal{C}$ or $\mathcal{B}$, $\omega \in \mathcal{P}$, and take $1 = A_1 \in \mathcal{C}_1$. Either $\rho(A_1) = 0$, in which case it follows from (4.10) that $\rho(\omega) = 0$, or we may write $\rho(A_1) = v^{-1}$, $v \in R_+^*$. In this case if $\rho(\chi_{p_1+1}) < v^{-1}\mu$ and

$$\rho(\omega) > v^{-1}(\alpha(p_2+1)p_2!/(p_2-p_1)! + \epsilon\mu),$$

we have

$$s(\mathcal{P}, \rho) \leq s((\chi, \omega, A_1), (\rho(\chi), \rho(\omega), v^{-1})) \leq v^{-1}F(v; w, \alpha). \quad (4.15)$$

Since for any choice of ϵ, $\alpha \in R_+^*$ the right-hand side of (4.15) tends to $-\infty$ when w tends to zero, this inequality implies that $\rho(\omega)$ tends to zero when w tends to zero. We have thus proved:

Proposition 4: Let U be a bounded open set of $R^{p\nu}$, $p \in N^*$ and let the correlation data $(\mathcal{P}, \rho)$ be compatible, where $\mathcal{P}$ is either $\mathcal{C}$ or $\mathcal{B}$. There exists then a function $w_U > 0$ of ϵ, defined for $\epsilon \in R_+^*$, such that if $\omega \in \mathcal{P} \cap \mathcal{C}_{p+1}$, $0 \leq \tilde{\omega} \leq 1$, and $\tilde{\omega}$ vanishes outside of a set of measure $\leq w$ with closure contained in U, then

$$\rho(\omega) \leq \epsilon \quad \text{if} \quad w \leq w_U(\epsilon). \quad (4.16)$$

Let $\mathcal{P} = \mathcal{C}$. If S is open, of Lebesgue measure $\leq w_U(\epsilon)$, and the closure of S is contained in U, we have, for the ρ measure of S,

$$\rho(S) \leq \epsilon. \quad (4.17)$$

Therefore if a subset of $R^{p\nu}$ is of Lebesgue measure zero, it is also of ρ-measure zero. By the Radon–Nikodym theorem[8] there exists thus a locally Lebesgue-integrable function $\tilde{\rho}_{p+1} \geq 0$ such that, for any $C \in \mathcal{C}_{p+1}$, $p \in N^*$, $\rho(C)$ is expressed by the following Lebesgue integral

$$\rho(C) = \int d\xi_1 \cdots d\xi_p \, \tilde{\rho}_{p+1}(\xi_1, \cdots, \xi_p) C(\xi_1, \cdots, \xi_p). \quad (4.18)$$

$\tilde{\rho}_{p+1}$ is defined only up to a set of measure zero, i.e., only its class ρ_{p+1} is determined. We will again note ρ the sequence $(\rho_{p+1})_{p \in N}$ and identify this sequence with an element of $\mathcal{K}$ (see Definition 4). We may then write, for any $C \in \mathcal{C}$,

$$\rho(C) = \int d\xi \, \tilde{\rho}(\xi) C(\xi) = \rho_1 C_1 + \sum_{p \in N^*} \int d\xi_1 \cdots d\xi_p \, \tilde{\rho}(\xi_1, \cdots, \xi_p) C(\xi_1, \cdots, \xi_p). \quad (4.19)$$

[8] See for instance L. H. Loomis, *An Introduction to Abstract Harmonic Analysis* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1953), p. 41.

We could have seen directly that $\tilde{\rho}$ is locally integrable by applying the Radon–Nicodym theorem to $\mathfrak{R}$ rather than $R^{p\nu}$.

Let now $\mathcal{P} = \mathfrak{B}$. If $B \in \mathfrak{B}_{p+1}$, $p \in N^*$ and $\tilde{B}$ vanishes outside of a closed set contained in the bounded open set U, it follows[9] from theorems of Lusin and Urysohn[4] that to any $w > 0$ there exists a function $C \subset \mathcal{C}_{p+1}$, with norm $||C|| \leq ||B||$ and support in U, such that $\tilde{B} - C$ vanishes outside of a set of Lebesgue measure $\leq w$. If $w \leq w_U(\epsilon)$ we have thus, using (4.18),

$$|\rho(B) - \rho(C)| < (||B|| + ||C||) \tag{4.20}$$

$$\left|\rho(C) - \int d\xi_1 \cdots d\xi_p \, \tilde{\rho}_{p+1}(\xi_1, \cdots, \xi_p)\tilde{B}(\xi_1, \cdots, \xi_p)\right| < \epsilon(||B|| + ||C||); \tag{4.21}$$

hence

$$\rho(B) = \int d\xi_1 \cdots d\xi_p \, \tilde{\rho}_{p+1}(\xi_1, \cdots, \xi_p)\tilde{B}(\xi_1, \cdots, \xi_p). \tag{4.22}$$

Theorem 2: If the correlation data $(\mathcal{P}, \rho)$ are compatible, where $\mathcal{P}$ is either $\mathcal{C}$ or $\mathfrak{B}$, there exists one and only one element of $\mathcal{K}$, again noted $\rho = (\rho_{p+1})_{p \in N}$ such that for all $A = (A_{p+1})_{p \in N} \in \mathcal{P}$,

$$\rho(A) = \int d\xi \, \tilde{\rho}(\xi)\tilde{A}(\xi) = \rho_1 A_1 + \sum_{p \in N^*} \int d\xi_1 \cdots d\xi_p \, \tilde{\rho}(\xi_1, \cdots, \xi_p)\tilde{A}(\xi_1, \cdots, \xi_p). \tag{4.23}$$

If $1 = A_1 \in \mathfrak{C}_1$ and $\rho(A_1) = 0$ we have seen that $\rho(A) = 0$ for all $A \in \mathcal{P}$ and it is easily checked that $s(\rho) = 0$.

5. CORRELATION FUNCTIONALS

If we put on $\mathcal{K}$ the topology of convergence in L^1 on the compacts, $\mathcal{K}$ becomes a Frechet space.[10] If the correlation data $(\mathcal{C}, \rho)$ or $(\mathfrak{B}, \rho)$ are compatible we have identified ρ with an element of $\mathcal{K}$. Using the bilinear form (4.22) we may identify the dual of $\mathcal{K}$ with $\mathfrak{B}$. $\mathfrak{B}$ with the strong topology $\mathfrak{I}_b[\mathcal{K}]$ is then identical to the inductive limit of the $\mathfrak{B}^K$ and induces on $\mathcal{C}$ the inductive limit topology of the $\mathcal{C}^K$, for which $\mathcal{C}$ is separable. We are however interested now in the weak topology $\mathfrak{I}_s[\mathcal{K}]$ of $\mathfrak{B}$. For this topology $\mathcal{C}$ is dense in $\mathfrak{B}$ and $\mathfrak{B}$ is thus separable.

Let now $\mathcal{P}_0$ be a countable weakly dense subset of $\mathfrak{B}$ such that for any compact $K \subset \mathfrak{R}$, with characteristic function $\tilde{\chi}^K$, there exists $A \in \mathcal{P}_0$ such that $\tilde{A} \geq \tilde{\chi}^K$. Let the correlation data $(\mathcal{P}_0, \rho_0)$ be compatible and write $s_0 = s(\mathcal{P}_0, \rho_0)$. Let X_1 and X_2 be subsets of $\mathfrak{B}$ containing $\mathcal{P}_0$ and χ_1, χ_2 extensions of ρ_0 to X_1 and X_2 respectively. If $X_1 \subset X_2$ and χ_2 is an extension of χ_1, we write $(X_1, \chi_1) \leq (X_2, \chi_2)$. With this order, the set of all couples (X, χ) of subsets of $\mathfrak{B}$ containing $\mathcal{P}_0$ and of extensions of ρ_0 such that that $s(X, \chi) = s_0$ is inductive. By Zorn's lemma it contains a maximal element $(\mathcal{P}, \rho)$.

We now see that $\mathcal{P} = \mathfrak{B}$. Let indeed $\mathbf{A}$ be a finite sequence of elements of $\mathcal{P}$ and $B \in \mathfrak{B}$. Define

$$I_{\mathbf{A}} = \{E : s((\mathbf{A}, B), (\rho(\mathbf{A}), E)) \geq s_0\}. \tag{5.1}$$

From Theorem 1 [the set $\{(\mathbf{E}, E) : s((\mathbf{A}, B), (\mathbf{E}, E)) \geq s_0\}$ is convex and closed] it follows that $I_{\mathbf{A}}$ is a closed interval. From the corollary to Theorem 1 and from Proposition 3 it follows that if $\mathbf{A}$ contains a function $\geq \tilde{\chi}^K$ where K contains the support of B, $I_{\mathbf{A}}$ is compact and not empty. If $\mathbf{A}$ is the sequence (A', A''), $I_{\mathbf{A}} \subset I_{\mathbf{A}'} \cap I_{\mathbf{A}''}$. In particular, no interval $I_{\mathbf{A}}$ is empty. The intersection I of all the intervals $I_{\mathbf{A}}$ being an intersection of closed sets with at least one compact cannot be empty, otherwise a finite intersection would already be empty and therefore one of the $I_{\mathbf{A}}$ would be empty. Therefore if $E_0 \in I$,

$$s((\mathbf{A}, B), (\rho(\mathbf{A}), E_0)) \geq s_0 \tag{5.2}$$

for any $\mathbf{A}$ and therefore

$$s(\mathcal{P} \cup \{B\}, \rho') = s_0, \tag{5.3}$$

where ρ' is the extension of ρ to $\mathcal{P} \cup \{B\}$ which takes the value E_0 at B. Since $(\mathcal{P}, \rho)$ is maximal, $B \in \mathcal{P}$, i.e., $\mathcal{P} = \mathfrak{B}$.

From Theorem 2 it follows then that ρ_0 must admit the weakly continuous linear extension ρ to $\mathfrak{B}$ and ρ is uniquely determined by ρ_0.

Proposition 5: Let $\mathcal{P}_0$ be a countable subset of $\mathfrak{B}$, dense in $\mathfrak{B}$ for its topology of weak dual of $\mathcal{K}$ and such that for any compact $K \subset \mathfrak{R}$, with characteristic function $\tilde{\chi}^K$, there exists $A \in \mathcal{P}_0$ such that $A \geq \chi^K$. Let the correlation data $(\mathcal{P}_0, \rho_0)$ be compatible. ρ_0 has then an extension to a linear functional $\rho \in \mathcal{K}$ on $\mathfrak{B}$ (this extension is unique). *The correlation data $(\mathfrak{B}, \rho)$ are compatible and we have*

$$s(\mathfrak{B}, \rho) = s(\mathcal{P}_0, \rho_0). \tag{5.4}$$

Corollary: If the correlation data $(\mathcal{C}, \rho_0)$ are compati-

[9] See for instance E. J. McShane, *Integration* (Princeton University Press, Princeton, New Jersey, 1947), pp. 236, 237.

[10] The relevant theorems for the properties quoted below can be found in G. Köthe, *Topologische Lineare Räume I* (Springer-Verlag, Berlin, 1960). What will be needed in the sequel is that, if $\mathfrak{B}$ is considered as a space of linear functionals on $\mathcal{K}$, there exists a countable subset of $\mathcal{C}$ which is dense in $\mathfrak{B}$ for the weak topology.

ble, where

$$\rho_0(C) = \int d\xi\ \tilde{\rho}(\xi)C(\xi), \tag{5.5}$$

then the correlation data $(\mathfrak{B}, \rho)$ *are compatible, with*

$$\rho(B) = \int d\xi\ \tilde{\rho}(\xi)\tilde{B}(\xi). \tag{5.6}$$

Furthermore

$$s(\mathfrak{B}, \rho) = s(\mathfrak{C}, \rho_0). \tag{5.7}$$

Definition 5: An element ρ *of* $\mathfrak{K}$ *such that the correlation data* $(\mathfrak{B}, \rho)$ *are compatible will be called a correlation functional and we will write* $s(\mathfrak{B}, \rho) = s(\rho)$.

Let $s(\mathbf{A}, \mathbf{I})$ be defined, where $\mathbf{A} = (A^\sigma)_{1\leq\sigma\leq q}$. If we write $A^\sigma = A^{\sigma+} - A^{\sigma-}$, $\sigma = 1, \cdots, q$, where $A^{\sigma+} \geq 0$, $A^{\sigma-} \geq 0$ (and $\tilde{A}^{\sigma-}$ does not take the value $+\infty$) we obtain from the corollary to Theorem 1 the relation

$$s(\mathbf{A}, \mathbf{I}) = s((\mathbf{A}, \mathbf{A}^+, \mathbf{A}^-), \mathbf{I} \times R^{2q}). \tag{5.8}$$

Hence, using Theorem 1 [Eq. (3.28)] and Proposition 3, to any $\epsilon \in R_+^*$ we may choose $\mathbf{I}^+$, $\mathbf{I}^-$ such that $\mathbf{I}^+ - \mathbf{I}^- \subset \mathbf{I}$ and

$$s((\mathbf{A}^+, \mathbf{A}^-), (\mathbf{I}^+, \mathbf{I}^-)) > s(\mathbf{A}, \mathbf{I}) - \epsilon. \tag{5.9}$$

We want to prove that we can find ρ such that $\rho(\mathbf{A}) \in \mathbf{I}$ and $s(\rho) > s(\mathbf{A}, \mathbf{I}) - 2\epsilon$. In view of the above remark it is sufficient to prove that ρ exists such that $\rho(\mathbf{A}^\pm) \in \mathbf{I}^\pm$ and $s(\rho) > s((\mathbf{A}^+, \mathbf{A}^-), (\mathbf{I}^+, \mathbf{I}^-)) - \epsilon$. In other words it is sufficient to show that ρ exists such that $\rho(\mathbf{A}) \in \mathbf{I}$ and $s(\rho) > s(\mathbf{A}, \mathbf{I}) - \epsilon$, supposing now $A^\sigma \geq 0$ for all σ.

Let thus $s(\mathbf{A}, \mathbf{I})$ be defined, $\mathbf{A} = (A^\sigma)_{1\leq\sigma\leq q}$ and $A^\sigma \geq 0$ for $\sigma = 1, \cdots, q$. Let also $\mathcal{P}_0$ be a subset of $\mathfrak{B}$ satisfying the conditions of Proposition 5 and $\mathbf{A}' = (A'^l)_{l\in N^*}$ be an infinite sequence of elements of $\mathfrak{A}$ containing all the elements of $\mathcal{P}_0$. We assume that, for all $l \in N^*$, $\tilde{A}'^l$ may take the value $+\infty$ only at points of $\mathfrak{R}$ for which some $\tilde{A}^\sigma$, $\sigma = 1, \cdots, q$, takes the value $+\infty$. We note $\mathbf{A}'_{(k)} = (A'^l)_{1\leq l\leq k}$, $k \in N^*$, the subsequence formed by the first k elements of $\mathbf{A}'$.

Given δ, $\epsilon \in R_+^*$ we may define, by recursion on k, sequences $\mathbf{I}_{(k)} \subset \mathbf{I}$ and $\mathbf{I}'_{(k)} \subset R^k$ of intervals of R satisfying the following conditions:

(1) The length of every interval of the sequences $\mathbf{I}_{(k)}$, $\mathbf{I}'_{(k)}$ is at most $k^{-1}\delta$.

(2) If the sequences $\mathbf{A}'_{(0)}$ and $\mathbf{I}'_{(0)}$ are defined to be empty and $\mathbf{I}_{(0)} = \mathbf{I}$, the closures of $\mathbf{I}_{(k)}$ and $\mathbf{I}'_k$ for $k \in N^*$ are contained in $\mathbf{I}_{(k-1)}$ and $\mathbf{I}'_{(k-1)} \times R$ respectively and the following inequality holds

$$s((\mathbf{A}, \mathbf{A}'_{(k)}), (\mathbf{I}_{(k)}, \mathbf{I}'_{(k)})) > s((\mathbf{A}, \mathbf{A}'_{(k-1)}), (\mathbf{I}_{(k-1)}, \mathbf{I}'_{(k-1)})) - 2^{-k}\epsilon. \tag{5.10}$$

That this is possible follows as above from the corollary of Theorem 1 and Eq. (3.28). The intersection over k of the $\mathbf{I}_{(k)}$ consists of only one point $\mathbf{E} \in \mathbf{I}$ and the intersection over k of the lth intervals of the $\mathbf{I}'_{(k)}$ consists of only one real number E'^l. Let $\mathbf{E}'_{(k)} = (E'^l)_{1\leq l\leq k}$. We have thus, for any k,

$$s((\mathbf{A}, \mathbf{A}'_{(k)}), (\mathbf{E}, \mathbf{E}'_{(k)})) > s(\mathbf{A}, \mathbf{I}) - \epsilon, \tag{5.11}$$

and it follows from Proposition 5 that there exists a correlation functional $\rho \in \mathfrak{K}$ such that, for all $A'^l \in \mathcal{P}_0$, $E'^l = \rho(A'^l)$.

We now show that we have

$$E^\sigma \geq \int d\xi\ \tilde{\rho}(\xi)\tilde{A}^\sigma(\xi) \tag{5.12}$$

for $\sigma = 1, \cdots, q$. For any $M \in N^*$ let indeed $\tilde{A}^{\sigma,M}$ be equal to $\tilde{A}^\sigma$ at the points of $\mathfrak{R}$ for which $\tilde{A}^\sigma \leq M$, equal to zero otherwise. We may assume that the classes $A^{\sigma,M}$ belong to $\mathcal{P}_0$, it follows then from Proposition 3 that

$$E^\sigma \geq \rho(A^{\sigma,M}) = \int d\xi\ \tilde{\rho}(\xi)\tilde{A}^{\sigma,M}(\xi) \tag{5.13}$$

and (5.12) follows from the theorem of B. Levi.[11]

Let us now assume that A' contains the square of A^σ for $\sigma = 1, \cdots, q$ [for definiteness we take $A'^\sigma = (A^\sigma)^2$] and also $A^\sigma - A^{\sigma,M}$, $(A^{\sigma,M})^2$, $A'^\sigma - (A^{\sigma,M})^2$ for all $M \in N^*$. Applying Proposition 3 to the inequality

$$(\tilde{A}^\sigma - \tilde{A}^{\sigma,M}) \leq M^{-1}((\tilde{A}^\sigma)^2 - (\tilde{A}^{\sigma,M})^2), \tag{5.14}$$

we obtain

$$E^\sigma - \int d\xi\ \tilde{\rho}(\xi)\tilde{A}^{\sigma,M}(\xi)$$

$$\leq M^{-1}\left(E'^\sigma - \int d\xi\ \tilde{\rho}(\xi)[\tilde{A}^{\sigma,M}(\xi)]^2\right) \leq M^{-1}E'^\sigma. \tag{5.15}$$

Letting M go to infinity we get

$$E^\sigma \leq \int d\xi\ \tilde{\rho}(\xi)\tilde{A}^\sigma(\xi). \tag{5.16}$$

Proposition 6: If $s(\mathbf{A}, \mathbf{I})$ *is defined,* $\mathbf{A} = (A^\sigma)_{1\leq\sigma\leq q}$, *to any* $\epsilon \in R_+^*$ *there exists a correlation functional* ρ *such that*

$$s(\rho) > s(\mathbf{A}, \mathbf{I}) - \epsilon \tag{5.17}$$

$$\int d\xi\ \tilde{\rho}(\xi)\tilde{A}^\sigma(\xi) \in I^\sigma \quad \text{for} \quad \sigma = 1, \cdots, q. \tag{5.18}$$

[11] See for instance F. Riesz and B. Sz-Nagy, *Leçons d'Analyse Fonctionnelle* (Académie des Sciences de Hongrie, Budapest, 1954), 3rd ed., p. 36.

6. CORRELATION FUNCTIONALS ASSOCIATED WITH FINITE CORRELATION DATA

Let ρ be a correlation functional and $\mathbf{A} = (A^\sigma)_{1\le\sigma\le q}$ a finite sequence of elements of $\mathfrak{A}$. Suppose that the functions $\tilde{\rho}\tilde{A}^\sigma$ are integrable on $\mathfrak{R}$ and that

$$E^\sigma = \int d\xi\, \tilde{\rho}(\xi)\tilde{A}(\xi)\, d\xi, \qquad \sigma = 1, \cdots, q. \quad (6.1)$$

We show that $s(\mathbf{A}, \mathbf{E}) \ge s(\rho)$, where $\mathbf{E} = (E^\sigma)_{1\le\sigma\le q}$. Since we may write $\tilde{A}^\sigma = \tilde{A}^{\sigma+} - \tilde{A}^{\sigma-}$, where $\tilde{A}^{\sigma+} \ge 0$, $\tilde{A}^{\sigma-} \ge 0$ and both $\tilde{\rho}\tilde{A}^{\sigma+}$ and $\tilde{\rho}\tilde{A}^{\sigma-}$ are integrable, it follows from Proposition 3 that it is sufficient to prove our statement under the assumption that $A^\sigma \ge 0$ for $\sigma = 1, \cdots, q$.

Let $\tilde{\chi}^M$, $M \in N^*$, be the characteristic function of the set of all $\xi \in \mathfrak{R}$ such that there exists a σ, $1 \le \sigma \le q$, for which $\tilde{A}^\sigma(\xi) > M$ or $\tilde{A}^\sigma(\xi) = +\infty$. Define also $\tilde{A}^{\sigma,M}(\xi) = \tilde{A}^\sigma(\xi)$ if $\tilde{A}^\sigma(\xi) \le M$, $\tilde{A}^{\sigma,M}(\xi) = 0$ otherwise. If $A^\sigma = (A^\sigma_{p+1})_{p\in N}\sigma = 1, \cdots, q$, there exists $r \in N^*$ such that $A^\sigma_{p+1} = 0$ for $p > r$. There exists also a compact $L \subset R^\nu$ such that for all σ and all p, the support of A^σ_{p+1} is contained in $(L)^p$. We call $\tilde{L}$ the characteristic function of L and write

$$\tilde{L}_{p+1}(\xi_1, \cdots, \xi_p) = \prod_{i=1}^{p} \tilde{L}_2(\xi_i). \quad (6.2)$$

For every $k \in N^*$ we construct a sequence $\mathbf{B}_{(k)} = (B^\sigma_{(k)})_{1\le\sigma\le kq+3}$ of elements of $\mathfrak{B}$ as follows: $1 = B^1_{(k)} \in \mathfrak{B}_1$, $B^2_{(k)}$ is the class of $\tilde{\chi}^k$, $B^3_{(k)}$ that of $\tilde{L}_{r+3}$, and $B^{q(M-1)+\sigma+3}_{(k)} = A^{\sigma,M}$ for $\sigma = 1, \cdots, q$; $M = 1, \cdots, k$. We define $\mathbf{E}_{(k)} = (E^\sigma_{(k)})_{1\le\sigma\le kq+3}$ by $E^\sigma_{(k)} = \rho(B^\sigma_{(k)})$ and let $\mathbf{I}_{(k)} = (I^\sigma_{(k)})_{1\le\sigma\le kq+3}$, $I^\sigma_{(k)} \ni E^\sigma_{(k)}$. By construction we have, for all k,

$$s(\mathbf{B}_{(k)}, \mathbf{I}_{(k)}) \ge s(\mathbf{B}_{(k)}, \mathbf{E}_{(k)}) \ge s(\rho) \quad (6.3)$$

and $t(v;\, \mathbf{B}_{(k)},\, v\mathbf{I}_{(k)})$ is therefore defined for some $v \in R^*_+$. It follows from the remarks after Theorem 1 and Theorem 2 that if $E^1_{(k)} = 0$ we have $s(\mathbf{A}, \mathbf{E}) \ge s(\rho) = 0$. We now assume that $E^1_k \in R^*_+$. Then, if the length of the interval $I^1_{(k)}$ is chosen sufficiently small, the function $t(v; B_{(k)}, vI_{(k)})$ of v will be defined only within an interval (v_0, v_1) of arbitrarily small length [with $v_0 < (E^1_{(k)})^{-1} < v_1$]. In particular to any $\delta \in R^*_+$ we may choose k so large and the intervals $I^1_{(k)}$ and $I^2_{(k)}$ such that $v_1 I^2_{(k)}$ is contained in the interval $(0, \delta)$ of R. We make use later of the possibility of choosing δ as small as we wish.

Given $\epsilon \in R^*_+$ we may choose $v (v_0 < v < v_1$, v possibly depending on $k)$ such that

$$t(v; B_{(k)}, vI_{(k)}) > v[s(\rho) - \epsilon]. \quad (6.4)$$

Let then $n \in N^*$ and $a = (a^i)_{1\le i\le\sigma} \in (R^*_+)^\nu$ be such that $n^{-1}V(a) = v$. For n large enough one may choose a such that

$$n^{-1} \log \mathfrak{V}' > v[s(\rho) - 2\epsilon], \quad (6.5)$$

where $n!\mathfrak{V}' = n!\mathfrak{V}'(\Lambda(a),\, n;\, \mathbf{B}_{(k)},\, v\mathbf{I}_{(k)})$ denotes the measure of the set $\mathfrak{p} \subset \Lambda'(a)^n$ of all X such that

$$n^{-1}\tilde{B}^\sigma[X] \in vI^\sigma, \qquad \sigma = 1, \cdots, kq + 3. \quad (6.6)$$

For every $X = (x_1, \cdots, x_n) \in \mathfrak{p}$ consider the elements x of the sequence X such that for some $p \in N^*$ there exist distinct elements $x_{i_1}, \cdots, x_{i_p}$ of X, distinct from x, such that

$$\tilde{\chi}^k_{p+1}(x_{i_1} - x, \cdots, x_{i_p} - x) = 1. \quad (6.7)$$

By suppressing all such elements x of X we obtain a sequence X' such that

$$\tilde{\chi}^k[X'] = 0. \quad (6.8)$$

X' consists of $n - n'$ elements, where $n' < n\delta$. Let $(n - n')!\mathfrak{V}'_{n-n'}$ be the measure of the subset of $\Lambda'(a)^{n-n'}$ consisting of sequences X' obtained as above. We have then

$$n!\mathfrak{V}' < \sum_{n'} \frac{n!}{n'!(n-n')!}\, V(a)^{n'}(n - n')!\mathfrak{V}'_{n-n'} \quad (6.9)$$

so that

$$\mathfrak{V}' < n\delta\left[\max_{0\le n'\le n\delta} \frac{V(a)^{n'}}{n'!}\right][\max_{n'} \mathfrak{V}'_{n-n'}]. \quad (6.10)$$

Therefore, for δ sufficiently small and n sufficiently large

$$n^{-1} \log \mathfrak{V}' < n^{-1} \log \mathfrak{V}'_{n-n''} + v\epsilon, \quad (6.11)$$

where n'' is the value of n' for which the maximum of $\mathfrak{V}'_{n-n'}$ occurs. From (6.5) and (6.11) we obtain

$$V(a)^{-1} \log \mathfrak{V}'_{n-n''} > s(\rho) - 3\epsilon. \quad (6.12)$$

Define now $n_l[X]$ as the number of elements x of the sequence X such that $x + L$ contains exactly l elements of X different from x. We have then

$$\tilde{L}_{p+1}[X] = \sum_{l\ge p} \frac{l!}{(l-p)!}\, n_l[X]. \quad (6.13)$$

We may choose $\gamma \in R^*_+$ (independently of k) such that $v_1 I^3_{(k)}$ is contained in the interval $(0, \gamma)$ of R. We have then

$$\sum_{l\le r+2} \frac{l!}{(l-r-2)!}\, n_l[X] < n\gamma. \quad (6.14)$$

Hence, for $p \le r$, $l \ge r + 2$

$$n^{-1}([l!/(l-p)!]n[X]) < [(l-r-2)!/(l-p)!]\gamma. \quad (6.15)$$

To any $\eta \in R_+^*$ one may thus choose $l_0 \in N^*$ such that

$$n^{-1} \sum_{l>l_0} \frac{l!}{(l-p)!} n_l[X] < \eta\gamma \quad \text{for} \quad p = 1, \cdots, r \tag{6.16}$$

and we obtain

$$\begin{aligned} & n^{-1}(\tilde{L}_{p+1}[X] - \tilde{L}_{p+1}[X']) \\ & < n^{-1} \sum_{l=p}^{l_0} \frac{l!}{(l-p)!} (n_l[X] - n_l[X']) + \eta\gamma \\ & \leq n^{-1} \frac{l_0!}{(l_0-p!)} \left[\sum_{l=p}^{l_0} (n_l[X] - n_l[X']) \right] + \eta\gamma \\ & \leq \delta l_0!/(l_0-p)! + \eta\gamma. \end{aligned} \tag{6.17}$$

The left-hand side is ≥ 0 and may be made arbitrarily small by taking δ sufficiently small.

Given $\theta \in R_+^*$ we may choose $M (M \in N^*, M \leq k)$ for k large enough such that $\rho(A^{\sigma,M}) > E^\sigma - \theta$ and take $I_{(k)}^{q(M-1)+\sigma+3} = (E^\sigma - \theta, E^\sigma + \theta)$ for $\sigma = 1, \cdots, q$. Then $\rho(A^{\sigma,k}) > E^\sigma - \theta$ and we may also take $I_{(k)}^{q(k-1)+\sigma+3} = (E^\sigma - \theta, E^\sigma + \theta)$. We have thus

$$\begin{aligned} & 0 \leq n^{-1}(\tilde{A}^{\sigma,M}[X] - \tilde{A}^{\sigma,M}[X']) \\ & \leq Mn^{-1}\left(n'' + \sum_{p=1}^{r} (\tilde{L}_{p+1}[X] - \tilde{L}_{p+1}[X'])\right) \\ & < M(\delta + r\delta l_0!/(l_0-r)! + r\eta\gamma) \end{aligned} \tag{6.18}$$

and we obtain for δ, η sufficiently small

$$\tilde{A}^{\sigma,M}[X'] \in V(a)I^\sigma \tag{6.19}$$

$$\tilde{A}^{\sigma,k}[X] \in V(a)I^\sigma, \tag{6.20}$$

where we have written $I^\sigma = (E^\sigma - 2\theta, E^\sigma + 2\theta)$. Finally from

$$\tilde{A}^{\sigma,M}[X'] \leq \tilde{A}^{\sigma,k}[X'] \leq \tilde{A}^{\sigma,k}[X] \tag{6.21}$$

$$\tilde{A}^\sigma[X'] = \tilde{A}^{\sigma,k}[X'], \tag{6.22}$$

we get

$$V(a)^{-1}\tilde{A}^\sigma[X'] \in I^\sigma. \tag{6.23}$$

Summing up, we have shown that, given $\epsilon, \theta \in R_+^*$, one can, for k sufficiently large, choose $n^* \in N$ such that for every $n \geq n^*$ there exists $n'' \in N$ and $a \in (R_+^*)^r$ satisfying the inequalities (6.12) and (6.23). Together these inequalities imply that

$$V(a)^{-1} \log \mathfrak{U}'(\Lambda(a); \mathbf{A}, \mathbf{I}) > s(\rho) - 3\epsilon, \tag{6.24}$$

where $\mathbf{I} = (I^\sigma)_{1 \leq \sigma \leq q}$. From this we get $s(\mathbf{A}, \mathbf{E}) \geq s(\rho)$.

Definition 6: Let $\rho \in \mathcal{K}$ be a correlation functional. If $A \in \mathcal{A}$ is such that $\tilde{\rho}\tilde{A}$ is integrable on $\mathfrak{R}$, we define

$$\rho(A) = \int d\xi\, \rho(\xi)\tilde{A}(\xi). \tag{6.25}$$

Proposition 7: If $\mathbf{A} = (A^\sigma)_{1 \leq \sigma \leq q}$ and $\rho(A^\sigma)$ is defined for all σ, $1 \leq \sigma \leq q$, then

$$s(\mathbf{A}, \rho(\mathbf{A})) \geq s(\rho). \tag{6.26}$$

Proposition 6 and Proposition 7 together imply the following result:

Theorem 3: $s(\mathbf{A}, \mathbf{I})$ is defined if and only if there exists a correlation functional ρ such that $\rho(\mathbf{A}) \in \mathbf{I}$, then,

$$s(\mathbf{A}, \mathbf{I}) = \sup_{\rho(\mathbf{A}) \in \mathbf{I}} s(\rho). \tag{6.27}$$

Let $P^* \subset R^q$ be the set of all $\mathbf{E}$ such that $\rho(\mathbf{A}) = \mathbf{E}$ for some correlation functional ρ. For $\mathbf{E} \in P^*$ we define

$$s^*(\mathbf{A}, \mathbf{E}) = \sup_{\rho(\mathbf{A}) = \mathbf{E}} s(\rho). \tag{6.28}$$

Theorem 3 then says that $s(\mathbf{A}, \mathbf{I})$ is defined if and only if $\mathbf{I} \cap P^* \neq \phi$ and that in that case

$$s(\mathbf{A}, \mathbf{I}) = \sup_{\mathbf{E} \in \mathbf{I} \cap P^*} s^*(\mathbf{A}, \mathbf{E}). \tag{6.29}$$

7. POSITIVITY AND BOUNDEDNESS PROPERTIES OF CORRELATION FUNCTIONS

It is convenient at this point to introduce a new space

$$\mathfrak{R} = \sum_{p+1 \in N} R^{(p+1)r},$$

with the same topology and measure as $\mathfrak{R}$, but to be considered as distinct from $\mathfrak{R}$. Let $\mathfrak{C}$ be the space of real continuous functions with compact support in $\mathfrak{R}$ and $\mathfrak{C}_{p+1}$ be the subspace of $\mathfrak{C}$ consisting of the functions with support in $R^{(p+1)r}$. $\mathfrak{C}$ is the direct sum of the $\mathfrak{C}_{p+1}$ and for any $f \in \mathfrak{C}$ we write $f = (f_{p+1})_{p+1 \in N}$ with $f_{p+1} \in \mathfrak{C}_{p+1}$, f_0 is identified to a real number.

Let $f_{p+1} \in \mathfrak{C}_{p+1}$, $p \in N$, and let ω be a partition of the set $\{0, 1, \cdots, p\}$ into r subsets $S_1 = \{i_{11}, i_{12}, \cdots\}, \cdots, S_r = \{i_{r1}, i_{r2}, \cdots\}$. We may suppose that $i_{jk} < i_{jk'}$ if $k < k'$ and $i_{j1} < i_{j'1}$ if $j < j'$. For all $Y = (y_1, \cdots, y_r) \in R^{rr}$, let $x_i^\omega(Y) = y_j$ if $i \in S_j$. We define $f_{(p+1)}^\omega \in \mathfrak{C}_r$ by

$$\begin{aligned} & f_{(p+1)}^\omega(y_1, \cdots, y_r) = f_{(p+1)}^\omega(Y) \\ & \quad = f_{p+1}(x_0^\omega(Y), x_1^\omega(Y), \cdots, x_p^\omega(Y)). \end{aligned} \tag{7.1}$$

The sum of the $f_{(p+1)}^\omega$ over all partitions of $\{0, 1, \cdots, p\}$ is an element $f_{(p+1)}$ of $\mathfrak{C}$. If $f = (f_{p+1})_{p+1 \in N} \in \mathfrak{C}$, we define $\Delta f \in \mathfrak{C}$ as

$$\Delta f = f_0 + \sum_{p \in N} f_{(p+1)}. \tag{7.2}$$

Let $\rho = (\rho_{p+1})_{p \in N} \in \mathcal{K}$ be a correlation functional.

We define a locally integrable function $\tilde{\varphi}$ on $\mathfrak{R}$ by the condition that it reduces to $\tilde{\varphi}_{p+1}$ on $R^{(p+1)\nu}$, $p+1 \in N$, where $\tilde{\varphi}_0 = 1$ and

$$\tilde{\varphi}_{p+1}(x_0, x_1, \cdots, x_p) = \rho_{p+1}(x_1 - x_0, \cdots, x_p - x_0) \tag{7.3}$$

for $p \in N$. Notice that, apart from a set of measure zero, $\tilde{\varphi}_{p+1}$ is, by definition of ρ, symmetric in its arguments $x_0, x_1, \cdots, x_p$. We introduce now a positive measure μ in $\mathfrak{R}$, i.e. a positive linear functional on $\mathfrak{C}$, by

$$\mu(f) = \int_{\mathfrak{R}} dx\, \tilde{\varphi}(x)\Delta f(x) = f_0 + \sum_{p\in N} \int dx_0\, dx_1 \cdots dx_p \times \tilde{\varphi}_{p+1}(x_0, x_1, \cdots, x_p)(\Delta f)_{p+1}(x_0, x_1, \cdots, x_p). \tag{7.4}$$

Let $f^1, f^2 \in \mathfrak{C}$, we define a structure of associative algebra over R in $\mathfrak{C}$ by introducing a product $f^1 \otimes f^2 \in \mathfrak{C}$ such that, for $p+1 \in N$,

$$(f^1 \otimes f^2)_{p+1}(x_0, x_1, \cdots, x_p) = \sum_{r+1=0}^{p+1} f^1_{r+1}(x_0, \cdots, x_r) f^2_{p-r}(x_{r+1}, \cdots, x_p). \tag{7.5}$$

From the symmetry property of the functions $\tilde{\varphi}_{p+1}$ it follows that if $f^j \in \mathfrak{C}$ for $j = 1, \cdots, m$, we have

$$\mu(f^1 \otimes \cdots \otimes f^j \otimes f^{j+1} \otimes \cdots \otimes f^m) = \mu(f^1 \otimes \cdots \otimes f^{j+1} \otimes f^j \otimes \cdots \otimes f^m). \tag{7.6}$$

If we define a linear mapping $\Theta : f \to C$ from $\mathfrak{C}$ to $\mathfrak{C}$, by writing

$$C_{p+1}(\xi_1, \cdots, \xi_p) = \int dx\, f_{p+1}(x, x+\xi_1, \cdots, x+\xi_p), \tag{7.7}$$

for $p \in N$, (7.4) becomes

$$\mu(f) = f_0 + \rho(\Theta\Delta f). \tag{7.8}$$

Let again $\Lambda'(a)$ be defined as the subset of $\Lambda(a)$ formed by the points x such that $x + \frac{1}{2}M \subset \Lambda(a)$, where

$$M = \{x : -\kappa \leq x^i \leq \kappa \text{ for } i = 1, \cdots, \nu\}, \tag{7.9}$$

but we assume now that κ is so chosen that f^j_{p+1} vanishes outside of $(\frac{1}{2}M)^{p+1}$, for $j = 1, \cdots, m$; $p \in N$. Let also $\tilde{\chi}_a$ be the characteristic function of $\Lambda(a)$. If $X = (x_1, \cdots, x_n) \in \Lambda'(a)^n$ and

$$f = \bigotimes_{j=1}^{m} f^j$$

we may write

$$\begin{aligned} f_0 + V(a)^{-1}(\Theta\Delta f)[X] &= V(a)^{-1}\left[f_0 V(a) + \sum_{p\in N}\sum_{i_0=1}^{n}\sum_{i_1=1}^{n}\cdots\sum_{i_p=1}^{n}(\Theta f)_{p+1}(x_{i_1} - x_{i_0}, \cdots, x_{i_p} - x_{i_0})\right] \\ &= V(a)^{-1}\int dx\left[\prod_{j=1}^{m}(f^j_0\tilde{\chi}_a(x)) + \sum_{p\in N}\sum_{i_0=1}^{n}\cdots\sum_{i_p=1}^{n}(f^1 \otimes \cdots \otimes f^m)_{p+1}(x + x_{i_0}, x + x_{i_1}, \cdots, x + x_{i_p})\right] \\ &= V(a)^{-1}\int dx \prod_{j=1}^{m}\left[f^j_0\tilde{\chi}_a(x) + \sum_{p\in N}\sum_{i_0=1}^{n}\cdots\sum_{i_p=1}^{n} f^j_{p+1}(x_{i_0} - x, x_{i_1} - x, \cdots, x_{i_p} - x)\right]. \end{aligned} \tag{7.10}$$

From this identity we obtain in particular that if $f^1, f^2 \in \mathfrak{C}$ and $f^2 \geq 0$, then

$$\mu(f^1 \otimes f^2 \otimes f^1) \geq 0. \tag{7.11}$$

Let $f^{\otimes m}$, $f \in \mathfrak{C}$, $m \in N^*$, be the mth power of f with respect to the product $\otimes$. If m is even, $m = 2r$, we define

$$||f||_{2r} = [\mu(f^{\otimes 2r})]^{1/2r}. \tag{7.12}$$

Then, the Hölder inequality yields

$$|\mu(f^1 \otimes f^2 \otimes \cdots \otimes f^{2r})| \leq \prod_{j=1}^{2r} ||f^j||_{2r}, \tag{7.13}$$

and the Minkowski inequality gives

$$||f^1 + f^2||_{2r} \leq ||f^1||_{2r} + ||f^2||_{2r}. \tag{7.14}$$

Let $f_1 \in \mathfrak{C}_1$, $f_1 \geq 0$ and $C_{p+1} = \Theta f_1^{\otimes(p+1)} \in \mathfrak{C}_{p+1}$ for some $p \in N$. If, for $x, y \in R'$ and $H = (\eta_1, \cdots, \eta_p)$, $(\xi_1, \cdots, \xi_p) \in R^{p\nu}$, we write

$$\tau_y f_1(x) = f_1(x - y) \tag{7.15}$$

$$\tau_H C_{p+1}(\xi_1, \cdots, \xi_p) = C_{p+1}(\xi_1 - \eta_1, \cdots, \xi_p - \eta_p), \tag{7.16}$$

we find

$$\begin{aligned} 0 \leq \rho(\tau_H C_{p+1}) &= \rho(\tau_H \Theta f_1^{\otimes p+1}) \\ &= \rho(\Theta(f_1 \otimes \tau_{\eta_1} f_1 \otimes \cdots \otimes \tau_{\eta_p} f_1)) \\ &\leq \rho(\Theta\Delta(f_1 \otimes \tau_{\eta_1} f_1 \otimes \cdots \otimes \tau_{\eta_p} f_1)) \\ &= \mu(f_1 \otimes \tau_{\eta_1} f_1 \otimes \cdots \otimes \tau_{\eta_p} f_1). \end{aligned} \tag{7.17}$$

On the other hand, applying the Hölder inequality

to (7.10), we obtain

$$\mu(f_1 \otimes \tau_{\eta_1} f_1 \otimes \cdots \otimes \tau_{\eta_p} f_1) \leq \mu(f_1^{\otimes p+1}) = \rho(\Theta \Delta f_1^{\otimes p+1}). \quad (7.18)$$

Writing $C = \Theta \Delta f_1^{\otimes (p+1)}$ we have thus

$$0 \leq \rho(\tau_H C_{p+1}) \leq \rho(C). \quad (7.19)$$

For any $B_{p+1} \in \mathfrak{B}_{p+1}$ one may choose f_1 such that $|B_{p+1}| \leq C_{p+1}$, then

$$|\rho(\tau_H B_{p+1})| \leq \rho(C). \quad (7.20)$$

We may reformulate our result as follows

Proposition 8: If $B_{p+1} \in \mathfrak{B}_{p+1}$ there exists $C \in \mathfrak{C}$, $C \geq 0$ such that, for any correlation functional ρ, the absolute value of the convolution product $\rho_{p+1} * B_{p+1}$ is bounded by $\rho(C)$.

$\rho_{p+1} * B_{p+1}$ is thus a continuous and bounded function.

8. INTRODUCTION OF A HILBERT SPACE[12]

It follows from (7.11) and more directly from (7.13), (7.14) that

$$|\mu(f^1 \otimes f^2)| \leq ||f^1||_2 \cdot ||f^2||_2, \quad (8.1)$$

$$||f^1 + f^2||_2 \leq ||f^1||_2 + ||f^2||_2. \quad (8.2)$$

Therefore, with respect to the scalar product $\mu(f^1 \otimes f^2)$, $\mathfrak{C}$ is a real pre-Hilbert space. Taking the quotient by the subspace[13] of the elements f^0 such that $||f^0||_2 = 0$ and then completing one obtains a real Hilbert space $\mathfrak{h}$. Let Ψ_f be the image of $f \in \mathfrak{C}$ in $\mathfrak{h}$, then the linear set D formed by all vectors Ψ_f is dense in $\mathfrak{h}$ by construction. Let $\mathfrak{C}^K$ be the subspace of $\mathfrak{C}$ formed by the functions f having their support in a compact $K \subset \mathfrak{R}$, and consider $\mathfrak{C}^K$ as a real Banach space with norm

$$||f|| = \max_{x \in K} |f(x)|. \quad (8.3)$$

The restriction of the mapping $f \to \Psi_f$ to $\mathfrak{C}^K$ is then continuous and $\mathfrak{h}$ therefore separable. The mapping $\Psi_f \to \Psi_{f^1 \otimes f}$ is linear and may be represented by an operator $Q(f^1)$ with domain D:

$$\Psi^1_{f \otimes f} = Q(f^1)\Psi_f. \quad (8.4)$$

[12] The Hilbert space construction described in this section follows Wightman's well-known construction in quantum field theory, see A. S. Wightman, Phys. Rev. **101**, 860 (1956) and also H. J. Borchers, Nuovo Cimento **24**, 214 (1962) and A. Uhlmann, Wiss. Zeitschr. Karl-Marx Univ. Leipzig. Math. Naturwiss. Reihe **11**, 213 (1962). The Wightman construction is itself analogous to Gelfand's construction (see for instance M. A. Naimark, *Normed Rings* (P. Noordhoff Ltd., Groningen, The Netherlands, 1959). Here however we may have a "degenerate vacuum" [cf. K. Hepp, R. Jost, D. Ruelle, and O. Steinmann, Helv. Phys. Acta **34**, 542 (1961)].

[13] This subspace is an ideal of the algebra $\mathfrak{C}$.

If $f^1 \geq 0$, then $Q(f^1) \geq 0$ by (7.11). If $\Phi, \Psi \in D$, $f^1, f^2 \in \mathfrak{C}$, we have

$$(\Phi, Q(f^1)\Psi) = (Q(f^1)\Phi, \Psi) \quad (8.5)$$

$$(\Phi, Q(f^1)Q(f^2)\Psi) = (\Phi, Q(f^2)Q(f^1)\Psi), \quad (8.6)$$

i.e., the operators $Q(f^1)$ are symmetric and commute with each other.

If $1 = f_0 \in \mathfrak{C}_0$, $Q(f_0)$ is the identity. If we write

$$\Psi_{f_0} = \Omega, \quad (8.7)$$

we have, for all $f \in \mathfrak{C}$,

$$\mu(f) = (\Omega, Q(f)\Omega). \quad (8.8)$$

Definition 7: For any $y \in R^\nu$, $f = (f_{p+1})_{p+1 \in N} \in \mathfrak{C}$, we define

$$\tau_y f_0 = f_0, \quad (8.9)$$

$$\tau_y f_{p+1}(x_0, x_1, \cdots, x_p) = f_{p+1}(x_0 - y, x_1 - y, \cdots, x_p - y), \quad p \in N, \quad (8.10)$$

$$\tau_y f = (\tau_y f_{p+1})_{p+1 \in N}. \quad (8.11)$$

The operator $U(y)$ defined by

$$U(y)\Psi_f = \Psi_{\tau_y f} \quad (8.12)$$

is unitary (or, since $\mathfrak{h}$ is real, orthogonal). The operators $U(y)$ define thus a strongly continuous unitary representation of the translation group of R^ν in $\mathfrak{h}$ (strong continuity follows from the continuity of the mapping $\mathfrak{C}^K \to D$ and the density of D in $\mathfrak{h}$). Notice that Ω is invariant under this representation.

Theorem 4. There exists a real separable Hilbert space $\mathfrak{h}$, a linear set D dense in $\mathfrak{h}$ and a linear mapping $f \to \Psi_f$ of $\mathfrak{C}$ onto D such that $(\Psi_{f^1}, \Psi_{f^2}) = \mu(f^1 \otimes f^2)$. The relation

$$Q(f^1)\Psi_f = \Psi_{f^1 \otimes f} \quad (8.13)$$

defines a symmetric linear operator $Q(f^1)$ with domain D, such that $Q(f^1)D \subset D$, $Q(f^1)Q(f^2) = Q(f^2)Q(f^1)$ and $f^1 \geq 0$ implies $Q(f^1) \geq 0$.

There exists a weakly continuous representation of the translation group of R^ν by unitary operators in $\mathfrak{h}$ which map D into itself, and a vector $\Omega \in D$ invariant under this representation and such that, for any $f \in \mathfrak{C}$,

$$Q(f)\Omega = \Psi_f, \qquad \mu(f) = (\Omega, Q(f)\Omega). \quad (8.14)$$

Let again $\tilde{\chi}_a$ be the characteristic function of $\Lambda(a)$, and let $f \in \mathfrak{C}$. We define

$$V(a)f_a = \int dy\, \tilde{\chi}_a(y)\tau_y f, \quad F(a) = ||V(a)f_a||_{2^\nu}. \quad (8.15)$$

It follows from (7.13) that

$$|\mu(\tau_{\nu_1} f \otimes \cdots \otimes \tau_{\nu_{2r}} f)| \leq [||f||_{2r}]^{2r} = \mu(f^{\otimes 2r}), \quad (8.16)$$

and from (7.14) that

$$F(a^1, \cdots, a'^i + a''^i, \cdots, a^r) \leq F(a^1, \cdots, a'^i, \cdots, a^r) + F(a^1, \cdots, a''^i, \cdots, a^r). \quad (8.17)$$

Lemma A1 (see Appendix), with N^* replaced by R_+^*, applies to the function $F(a)$ because of (8.17) and the boundedness property (8.16). There exists therefore $S \in R_+$ such that, when $a \to \infty$ (i.e., $\min_{1\leq i\leq r} a^i \to +\infty$),

$$\lim F(a)/V(a) = \inf F(a)/V(a) = S^{1/2r}. \quad (8.18)$$

This means that $\mu(f_a^{\otimes 2r})$ has the limit S.

Let now $f^j \in \mathfrak{C}$, $1 \leq j \leq 2r$. We have the identities

$$\sum_{\epsilon_2=\pm 1} \cdots \sum_{\epsilon_{2r}=\pm 1} \left(\prod_{j=2}^{2r} \epsilon_j\right) \mu\left(\left(f_a^1 + \sum_{j=2}^{2r} \epsilon_j f_a^j\right)^{\otimes 2r}\right) = (2r)!\, 2^{2r-1} \mu(f_a^1 \otimes \cdots \otimes f_a^{2r}) \quad (8.19)$$

$$f_a^1 + \sum_{j=2}^{2r} \epsilon_j f_a^j = \left(f^1 + \sum_{j=2}^{2r} \epsilon_j f^j\right)_a. \quad (8.20)$$

Therefore, when $a \to \infty$,

$$\lim \mu(f_a^1 \otimes \cdots \otimes f_a^{2r}) = S', \quad (8.21)$$

with $S' \in R$. From (8.15) and (7.13) we have

$$\mu(f_a^1 \otimes \cdots \otimes f_a^{2r}) = V(a)^{-2r} \int dy_1 \cdots dy_{2r} \times \tilde{\chi}_a(y_1) \cdots \tilde{\chi}_a(y_{2r}) \mu(\tau_{y_1} f^1 \otimes \cdots \otimes \tau_{y_{2r}} f^{2r}), \quad (8.22)$$

$$|\mu(\tau_{y_1} f^1 \otimes \cdots \otimes \tau_{y_{2r}} f^{2r})| \leq \prod_{j=1}^{2r} ||f^j||_{2r}, \quad (8.23)$$

which implies that, if $\eta_j \in R^r$ for $j = 1, \cdots, 2r$,

$$\lim_{a\to\infty} \mu(\tau_{\eta_1} f_a^1 \otimes \cdots \otimes \tau_{\eta_{2r}} f_a^{2r}) = \lim_{a\to\infty} \mu(f_a^1 \otimes \cdots \otimes f_a^{2r}) = S'. \quad (8.24)$$

Notice also that, if $1 = f^{2r} \in \mathfrak{C}_0$,

$$\mu(f_a^1 \otimes \cdots \otimes f_a^{2r}) = \mu(f_a^1 \otimes \cdots \otimes f_a^{2r-1}). \quad (8.25)$$

(8.21) and (8.24) hold therefore with $2r$ replaced by any integer m.

We may at this point construct from the expressions S' a Hilbert space $\mathfrak{h}'$ and operators Q' in a manner similar[14] to that in which we constructed $\mathfrak{h}$ and the operators Q from the expressions $\mu(f)$.

Proposition 9: There exist a real separable Hilbert space $\mathfrak{h}'$, a linear set D' dense in $\mathfrak{h}'$, a vector $\Omega' \in D'$ and, for every $f \in \mathfrak{C}$, a symmetric operator $Q'(f)$ with domain D' such that $Q'(f)D' \subset D'$, $Q'(f^1)Q'(f^2) = Q'(f^2)Q'(f^1)$ and $f \geq 0$ implies $Q(f) \geq 0$. If $\tilde{\chi}_a$ is the characteristic function of $\Lambda(a)$ and we write

$$f_a = V(a)^{-1} \int dy\, \tilde{\chi}_a(y) \tau_y f; \quad (8.26)$$

then, when $\min_{1\leq i\leq r} a^i \to +\infty$,

$$\lim \mu(f_a^1 \otimes \cdots \otimes f_a^m) = (\Omega', Q'(f^1) \cdots Q'(f^m)\Omega'). \quad (8.27)$$

Furthermore,

$$Q'(\tau_y f) = Q'(f) \quad (8.28)$$

$$(\Omega', Q'(f)\Omega') = (\Omega, Q(f)\Omega) = \mu(f). \quad (8.29)$$

Here D' is the set of vectors $P\Omega'$ of $\mathfrak{h}'$ obtained by applying a polynomial P in the operators $Q'(f)$ to Ω'.

9. ANALYTIC CORRELATION FUNCTIONALS

Definition 8: The correlation functional ρ is said to be analytic if, for each $f \in \mathfrak{C}$,

$$\limsup_{m\to\infty} \left[\frac{1}{m!} K_m(f)\right]^{1/m} \in R_+ \quad (9.1)$$

where

$$K_m(f) = \sup_{\nu_1, \cdots, \nu_m} |\rho(\Theta(\tau_{\nu_1} f \otimes \cdots \otimes \tau_{\nu_m} f))|. \quad (9.2)$$

Let $f = (f_{p+1})_{p+1\in N}$, $f_{p+1} = 0$ for $p \geq r$. It is sufficient to check (9.1) when $f_0 = 0$. One may then find $g_1 \in \mathfrak{C}_1$, $g_1 \geq 0$ such that $|f_{p+1}| \leq g_1^{\otimes(p+1)}$ for $p = 0, \cdots, r-1$. In that case

$$K_m(f) \leq r^m \max_{m\leq m'\leq rm} K_{m'}(g_1). \quad (9.3)$$

In particular (9.1) is satisfied if, for some $D \in R_+^*$ and all $m \in N^*$,

$$K_m(g_1) \leq D^m. \quad (9.4)$$

Let $f^j \in \mathfrak{C}_{p_j+1}$, $p_j \in N$, $j = 1, \cdots, m$. We have

$$(\Omega', Q'(f^1) \cdots Q'(f^m)\Omega) = \lim_{a\to\infty} V(a)^{-m} \int dy_1 \cdots dy_m \times \tilde{\chi}_a(y_1) \cdots \tilde{\chi}_a(y_m) \rho(\Theta\Delta(\tau_{y_1} f^1 \otimes \cdots \otimes \tau_{y_m} f^m). \quad (9.5)$$

The expression $\Delta(\tau_{y_1} f^1 \otimes \cdots \otimes \tau_{y_m} f^m)$ is a sum over the partitions of the set $\{0, 1, \cdots, \sum_{i=1}^m (p_i+1) - 1\}$. Consider a partition ω which is not finer than the partition into the subsets

$$S_j = \left\{\sum_{i=1}^{j-1} (p_i + 1), \cdots, \sum_{i=1}^{j} (p_i + 1) - 1\right\}, \quad j = 1, \cdots, m.$$

[14] The role of the algebra $\mathfrak{C}$ being now played by the tensor algebra of $\mathfrak{C}$ considered as real vector space.

This means that there is a set S in the partition ω such that S contains elements of S_{j_1} and S_{j_2}, $j_1 \neq j_2$. The term

$$\rho(\Theta(\tau_{y_1} f^1 \otimes \cdots \otimes \tau_{y_m} f^m)^\omega) \tag{9.6}$$

is, by Proposition 8, a bounded function of $y_1, \cdots, y_m$, and it vanishes if $y_{j_2} - y_{j_1}$ is outside of some compact in R^ν. This implies that the contribution of (9.6) to (9.5) vanishes and we may write

$$(\Omega', Q'(f^1) \cdots Q'(f^m)\Omega')$$

$$= \lim_{a\to\infty} V(a)^{-m} \int dy_1 \cdots dy_m\, \tilde{\chi}_a(y_1) \cdots \tilde{\chi}_a(y_m)$$

$$\times \rho(\Theta(\tau_{y_1} \Delta f^1 \otimes \cdots \otimes \tau_{y_m} \Delta f^m)). \tag{9.7}$$

Obviously this formula remains true for any $f^j \in \mathfrak{C}$, $j = 1, \cdots, m$. In particular, for $f = f^1 = \cdots = f^m$ we obtain

$$|(\Omega', Q'(f)^m \Omega')| \leq K_m(\Delta f). \tag{9.8}$$

Let $f^1, f^2, \cdots, \in \mathfrak{C}$ and let $\Psi = P\Omega' \in D'$ where P is a polynomial in the operators $Q'(f^1)$, $Q'(f^2)$, $\cdots$. We have

$$|(\Psi, Q'(f)^m \Psi)| = |(P^2\Omega', Q'(f)^m \Omega')|$$

$$\leq (\Omega', P^4\Omega')^{\frac{1}{2}} (\Omega', Q'(f)^{2m}\Omega')^{\frac{1}{2}}. \tag{9.9}$$

If ρ is an analytic correlation functional

$$\limsup_{m\to\infty} \left[\frac{1}{m!} (\Omega', Q'(f)^{2m}\Omega')^{\frac{1}{2}}\right]^{1/m}$$

$$= 2 \limsup_{m\to\infty} \left[\frac{1}{(2m)!} (\Omega', Q'(f)^{2m}\Omega')\right]^{1/2m}$$

$$\leq 2 \limsup_{m\to\infty} \left[\frac{1}{m!} K_m(\Delta f)\right]^{1/m} \in R_+, \tag{9.10}$$

and therefore the power series

$$\sum_{m=0}^{\infty} ||Q'(f)^m \Psi|| \frac{z^m}{m!} \tag{9.11}$$

has a nonvanishing radius of convergence. Every vector Ψ in the domain D' of every operator $Q'(f)$, $f \in \mathfrak{C}$, is thus an analytic vector (in the sense of Nelson[15a]) for this operator. From this follows[15b] that the operators $Q'(f)$ are essentially self-adjoint. Let $\bar{Q}'(f)$ be their closures. If $f^1, f^2 \in \mathfrak{C}$, $f^1 \geq 0$, $f^2 \geq 0$ and $\Psi \in (1 + Q'(f^1))(1 + Q'(f^2))D'$, we have

$$(1 + \bar{Q}'(f^1))^{-1}(1 + \bar{Q}'(f^2))^{-1}\Psi$$

$$= (1 + \bar{Q}'(f^2))^{-1}(1 + \bar{Q}'(f^1))^{-1}\Psi. \tag{9.12}$$

Since $Q'(f^2)$ is essentially self-adjoint on D', $(1 + Q'(f^2))D'$ is dense in $\mathfrak{h}'$ and the restriction of $Q'(f^1)$ to $(1 + Q'(f^2))D'$ is essentially self-adjoint. Therefore $(1 + Q'(f^1))(1 + Q'(f^2))D'$ is dense in $\mathfrak{h}$ and the bounded operators $(1 + \bar{Q}'(f^1))^{-1}$ and $(1 + \bar{Q}'(f^2))^{-1}$ commute. This means that the spectral projections of $\bar{Q}'(f^1)$ and $\bar{Q}'(f^2)$ commute, and this remains true obviously for any $f^1, f^2 \in \mathfrak{C}$.

Proposition 10: If ρ is an analytic correlation functional, the operators $Q'(f)$, $f \in \mathfrak{C}$, are essentially self-adjoint and the spectral projections of their closures $\bar{Q}'(f)$ commute.

10. EXISTENCE OF A THERMODYNAMIC LIMIT

Let Φ be a two-body central potential (for definiteness), i.e., a measurable function on R^ν, with values in $R \cup \{+\infty\}$, such that $\Phi(\xi) = \Phi(\eta)$ if $|\xi| = |\eta|$, where

$$|\xi| = \left(\sum_{i=1}^{\nu} (\xi^i)^2\right)^{\frac{1}{2}}.$$

We assume that Φ has a hard core [i.e., $\Phi(\xi) = +\infty$ if and only if $|\xi| < d$, $d \in R_+^*$] and finite range (i.e., compact support). We also assume that Φ takes only the value $+\infty$ and values in a bounded interval of R. Consider a system of identical particles enclosed in a box $\Lambda(a)$ and interacting through Φ at temperature β^{-1} ($\beta \in R_+^*$). The grand canonical formalism prescribes that to each configuration of n particles in $\Lambda(a)$, with positions $x_1, \cdots, x_n$, a weight

$$z^n e^{-\beta U(x)_n} \tag{10.1}$$

be associated, where $z = e^{\beta\bar{\mu}}$ is the activity ($\bar{\mu} \in R$) and

$$U(x)_n = \sum_{1\leq i\leq j\leq n} \Phi(x_i - x_j). \tag{10.2}$$

We consider the particles in a configuration as unlabeled, hence the total weight is[16]

$$\Xi_a = \sum_{n\in N} \frac{z^n}{n!} \int_{\Lambda(a)^n} dx_1 \cdots dx_n\, e^{-\beta U(x)_n}. \tag{10.3}$$

Let $\mathbf{A} = (A^\sigma)_{\sigma\in N^*}$ be an infinite sequence of elements of $\mathfrak{A}$ such that

(1) $A_1^1 = -\bar{\mu}$, $A_2^1 = \frac{1}{2}\Phi$ and $A_{p+1}^1 = 0$ for $p > 1$.

(2) $A^\sigma \in \mathfrak{C}$ if $\sigma > 1$ and any $C \in \mathfrak{C}$ may be approximated uniformly by linear combinations of A^σ, $\sigma > 1$, with supports in a fixed compact.

[15] (a) E. Nelson, Ann. Math. **70**, 572 (1959). (b) Ref. 15(a), Sec. 5, Lemma 5.1. Let us note that the proof of this lemma does not make use of the results in Secs. 1–4. of Nelson's paper, and may be studied independently. An application of Nelson's lemma to a situation somewhat analogous to that considered here has been made by H. J. Borchers and W. Zimmermann, Nuovo Cimento **31**, 1047 (1964).

[16] Whether the sum in (10.3) is extended over $n \in N$ or $n \in N^*$ is of no importance in the limits which will be taken.

(3) For any compact $K \subset \mathfrak{R}$ with characteristic function $\tilde{\chi}^K$, there exists $\sigma > 1$ such that $A^\sigma \geq \chi^K$. It follows from (2) and (3) that $\mathcal{O}_0 = \{A^\sigma : \sigma > 1\}$ satisfies the conditions of Proposition 5. We note $\mathbf{A}_{(q)} = (A^\sigma)_{1\leq\sigma\leq q}$, $q \in N^*$, the subsequence formed by the first q elements of $\mathbf{A}$.

For any given q, we may choose κ [see (1.7)] relatively to the sequence $\mathbf{A}_{(q)}$ and define the symbol Λ'. Let then $b \in (R_+^*)^\nu$ be such that $\Lambda'(b)$ is a translate of $\Lambda(a)$. Let $\mathbf{I}_{(q)} = (I^\sigma)_{1\leq\sigma\leq q}$, we have for the contribution $\Xi_a(\mathbf{I}_{(q)})$ to Ξ_a of the configurations X such that

$$V(b)^{-1}\tilde{A}[\chi] \in I^\sigma, \qquad \sigma = 1, \cdots, q, \tag{10.4}$$

the relation

$$\Xi_a(\mathbf{I}_{(q)}) \in \mathfrak{U}'(\Lambda(b); \mathbf{A}_{(q)}, \mathbf{I}_{(q)})e^{-\beta V(b)I^1}. \tag{10.5}$$

If $\beta I^1 \subset (\beta E^1 - \epsilon, \beta E^1 + \epsilon)$ with $E^1 \in R$, $\epsilon \in R_+^*$, we obtain thus, using (3.21),

$$s(\mathbf{A}_{(q)}, \mathbf{I}_{(q)}) - \beta E^1 - 2\epsilon < V(b)^{-1} \log \Xi_a(\mathbf{I}_{(q)}) < s(\mathbf{A}_{(q)}, \mathbf{I}_{(q)}) - \beta E^1 + 2\epsilon, \tag{10.6}$$

when $\min_{1\leq i\leq\nu} a^i$ is large enough. It follows from our assumptions on Φ that the domain of definition of $s(\mathbf{A}_{(q)}, \mathbf{E})$ in R^q is bounded. (10.6) implies thus for the grand canonical expression of the pressure

$$\beta^{-1} \lim_{a\to\infty} V(a)^{-1} \log \Xi_a = \max_{\mathbf{E}} [\beta^{-1}s(\mathbf{A}_{(q)}, \mathbf{E}) - E^1], \tag{10.7}$$

where the values of $\mathbf{E} = (E^\sigma)_{1\leq\sigma\leq q}$ for which the maximum is obtained in the right-hand side form a nonempty convex compact set $K_{(q)} \subset R^q$.

Consider now the grand canonical correlation functions defined for $p \in N^*$ by

$$\tilde{\varphi}_{a,p}(x_1, \cdots, x_p) = \Xi_a^{-1} \sum_{n\in N} \frac{z^{p+n}}{n!} \times \int dx_{p+1} \cdots dx_{p+n} \prod_{i=1}^{p+n} \tilde{\chi}_a(x_i) e^{-\beta U(x)_{p+n}}, \tag{10.8}$$

where $\tilde{\chi}_a$ is the characteristic function of $\Lambda(a)$. We replace them by the "averaged" functions

$$\tilde{\rho}_{a,p+1}(\xi_1, \cdots, \xi_p) = V(a)^{-1} \times \int dx\, \tilde{\varphi}_{a,p+1}(x, x + \xi_1, \cdots, x + \xi_p) \tag{10.9}$$

(with $p \in N$) and define for all $\sigma \in N^*$

$$E^\sigma(a) = \sum_{p\in N} \int d\xi_1 \cdots d\xi_p \times \tilde{A}^\sigma_{p+1}(\xi_1, \cdots, \xi_p)\tilde{\rho}_{a,p+1}(\xi_1, \cdots, \xi_p)$$

$$= \Xi_a^{-1} \sum_{n\in N} \frac{z^n}{n!} \int dx_1 \cdots dx_n \times \prod_{i=1}^{n} \tilde{\chi}_a(x_i) V(a)^{-1} \tilde{A}^\sigma[X] e^{-\beta U(x)_n}. \tag{10.10}$$

It is then easily seen that $\mathbf{E}_{(q)}(a) = (E^\sigma(a))_{1\leq\sigma\leq q}$ will belong to any neighborhood of $K_{(q)}$ if $\min_{1\leq i\leq\nu} a^i$ is large enough.

Let $(a_j)_{j\in N}$ be a sequence of elements of $(R_+^*)^\nu$ such that $\lim_{j\to\infty} a_i^j = +\infty$ for $i = 1, \cdots, \nu$. Taking successively $q = 1, 2, \cdots$, we may by a diagonal procedure extract from $(a_j)_{j\in N}$ a sequence $(a'_j)_{j\in N}$ such that

$$\lim_{j\to\infty} \mathbf{E}_{(q)}(a'_j) = \mathbf{E}'_{(q)} \in K_{(q)} \tag{10.11}$$

for all $q \in N^*$. Let $\mathbf{E}'_{(q)} = (E'^\sigma)_{1\leq\sigma\leq q}$. Since $\mathbf{E}'_{(q)} \in K_{(q)}$ there exists, by Proposition 5, a correlation functional ρ such that $\rho(A^\sigma) = E'^\sigma$ for $\sigma \in N^*$ and, by Proposition 7 and (10.7),

$$\beta^{-1} \lim_{j\to\infty} V(a'_j)^{-1} \log \Xi_{a'_j} = \beta^{-1}s(\rho) - E'^1. \tag{10.12}$$

Because of our assumptions on Φ, there exists $D \in R_+^*$ such that

$$\tilde{\varphi}_{a,p+1} \leq D^{p+1}, \qquad \tilde{\rho}_{a,p+1} \leq D^{p+1} \tag{10.13}$$

for all $p \in N$ and $a \in (R_+^*)^\nu$. The Assumption 2 on the sequence $\mathbf{A}$ then implies that, when $j \to \infty$, $\rho_{a'_j,p+1}$ converges weakly on $\mathfrak{C}_{p+1}$ towards ρ_{p+1} for all $p \in N$, and

$$\rho_{p+1} \leq D^{p+1}. \tag{10.14}$$

Using Lusin's theorem as in the proof of Theorem 2, one sees that $\rho_{a'_j,p+1}$ also converges weakly on $\mathfrak{B}_{p+1}$ towards ρ_{p+1}. (10.14) implies that ρ is an analytic correlation functional.

Proposition A: Let the central two-body potential Φ have finite range and take only the value $+\infty$ and values in a bounded interval of the real axis. Let $\beta > 0, z > 0$ and let Λ_j, $j = 1, 2, \cdots$ be a sequence of parallelopipeds with volumes V_j in ν dimensions such that the smallest side of Λ_j tends to infinity when $j \to \infty$. Define

$$U(x)_n = \sum_{1\leq i<j\leq n} \Phi(x_j - x_i), \tag{10.15}$$

$$\Xi_j = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\Lambda_j} dx_1 \cdots \int_{\Lambda_j} dx_n\, e^{-\beta U(x)_n}, \tag{10.16}$$

$$\tilde{\varphi}^j_p(x_1, \cdots, x_p) = \Xi_j^{-1} \sum_{n=0}^{\infty} \frac{z^{p+n}}{n!} \times \int dx_{p+1} \cdots dx_{p+n} \prod_{i=1}^{p+n} \tilde{\chi}_j(x_i) e^{-\beta U(x)_{p+n}}, \tag{10.17}$$

$$\tilde{\rho}^i_{p+1}(\xi_1, \cdots, \xi_p)$$

$$= V_i^{-1} \int dx\, \tilde{\varphi}^i_{p+1}(x, x+\xi_1, \cdots, x+\xi_p), \quad (10.18)$$

where $\tilde{\chi}_i$ is the function equal to 1 inside of Λ_i, to zero outside. Then, one may choose a subsequence $\tilde{\rho}'^i$, $j = 1, 2, \cdots$, of the sequence of the ρ^i such that for every $p \geq 0$ and every bounded Lebesgue-measurable function $\tilde{B}$, of p ν-dimensional vectors, vanishing outside of a bounded region,

$$\lim_{i\to\infty} \beta^{-1} V_i^{-1} \log \Xi_i = P, \quad (10.19)$$

$$\lim_{i\to\infty} \int d\xi_1 \cdots d\xi_p\, \tilde{\rho}'^i_{p+1}(\xi_1, \cdots, \xi_p)\tilde{B}(\xi_1, \cdots, \xi_p)$$

$$= \int d\xi_1 \cdots d\xi_p\, \tilde{\rho}_{p+1}(\xi_1, \cdots, \xi_p)\tilde{B}(\xi_1, \cdots, \xi_p), \quad (10.20)$$

where P is a real number ≥ 0 and $\tilde{\rho}_{p+1}$ is a bounded Lebesgue-measurable function ($p = 1, 2, \cdots$). The sequence $\rho = (\rho_{p+1})_{p\in N}$ is an analytic correlation functional and

$$P = \beta^{-1} s(\rho) + \rho_1 \bar{\mu} - \frac{1}{2} \int d\xi\, \rho_2(\xi)\Phi(\xi). \quad (10.21)$$

11. THE PROBLEM OF EXISTENCE OF PHASES

As we have seen, statistical mechanics leads typically to consider configurations of a large number of points $(x_1, \cdots, x_n)$ in a large region $\Lambda(a) \subset R^\nu$ satisfying conditions of the form $V(a)^{-1}\tilde{A}[X] \in I$, where I shrinks to a point in the limit. The main objective of this paper was to show that, among these configurations, most satisfy other conditions of the same type, so that the correlations between the points of the configuration are strictly determined, and should be given by a correlation functional. A typical result in this direction was given in Sec. 10. Of course one does not expect physically that to a given set of data of the form $V(a)^{-1}\tilde{A}[X] \approx E$ there will always correspond only one correlation functional, there may be several or even, for "unphysical" data, none at all [for instance, in Eq. (6.28), the supremum may not be attained].

Let us now investigate the macroscopic aspect of a large configuration of points with correlations approximating those determined by an analytic functional ρ.

Proposition B: Let $(a_j)_{j\in N}$ and $(\kappa_j)_{j\in N}$ be sequences of elements of $(R^*_+)^\nu$ and R^*_+ respectively, such that when $j \to \infty$, then $\kappa_j \to \infty$ and $\kappa_j^{-1} a_j^i \to \infty$ for $i = 1, \cdots, \nu$. Define

$$M_j = \{x : -\kappa_j < x^i < \kappa_j \text{ for } i = 1, \cdots, \nu\}, \quad (11.1)$$

$$\Lambda'_j = \{x : x + M_j \in \Lambda(a_j)\}. \quad (11.2)$$

For each $j \in N$, let $X_j = (x_{j1}, \cdots, x_{jn_j})$ be a sequence of elements of Λ'_j. We assume that for each $f \in \mathfrak{C}$,

$$\lim_{j\to\infty} V(a_j)^{-1} \int_{\Lambda(a_j)} dx\, f_{X_j}(x) = \mu(f), \quad (11.3)$$

where μ is the measure on $\mathfrak{N}$ associated with an analytic correlation functional ρ and

$$f_{X_j}(x) \quad f_0 + \sum_{p\in N} \sum_{i_0=1}^{n_j} \cdots \sum_{i_p=1}^{n_j} f(x + x_{ji_0}, \cdots, x + x_{ji_p}). \quad (11.4)$$

Under the above conditions one can choose a sequence $(c_j)_{j\in N}$ of elements of $(R^*_+)^\nu$ such that

$$\lim_{j\to\infty} c_j^i = +\infty \text{ for } i = 1, \cdots, n;\ c_j^i < \tfrac{1}{2}\kappa_j, \quad (11.5)$$

and for every real continuous function φ with compact support in R^q, $q \in N^*$, and every q-tuple $f^1, \cdots, f^q$ of elements of $\mathfrak{C}$,

$$\lim_{j\to\infty} (\zeta_j(f^1_{c_j}, \cdots, f^q_{c_j}))(\varphi)$$

$$= \left(\Omega', \varphi(\tilde{Q}'(f^1), \cdots, \tilde{Q}'(f^q))\Omega'\right), \quad (11.6)$$

where f_c is defined by (8.26) and the measure $\zeta_j(f^1, \cdots, f^q)$ on R^q is defined by

$$(\zeta_j(f^1, \cdots, f^q))(\varphi)$$

$$= V(a_j)^{-1} \int_{\Lambda(a_j)} dx\, \varphi(f^1_{X_j}(x), \cdots, f_{X_j}(x)). \quad (11.7)$$

Notice that a sequence $(X_j)_{j\in N}$ satisfies (11.3) for all $\mathfrak{C}$ if it satisfies this condition for a suitable countable subset of $\mathfrak{C}$. One may in particular construct $(X_j)_{j\in N}$ with "typical" configurations occuring in Proposition A.

To prove Proposition B notice that all the moments of the measures $\zeta_j(f^1, \cdots, f^j)$ exist and, using a functional notation for measures we have, for all $r_1, \cdots, r_q \in N$,

$$\lim_{j\to\infty} \int_{-\infty}^{\infty} d\alpha_1 \cdots \int_{-\infty}^{\infty} d\alpha_q\, \alpha_1^{r_1} \cdots \alpha_q^{r_q}(\zeta_j(f^1, \cdots, f^q))$$

$$\cdot (\alpha_1, \cdots, \alpha_q) = \mu((f^1)^{\otimes r_1} \otimes \cdots \otimes (f^r)^{\otimes r_q}). \quad (11.8)$$

Therefore

$$\lim_{c\to\infty} \lim_{j\to\infty} \int_{-\infty}^{\infty} d\alpha_1 \cdots \int_{-\infty}^{\infty} d\alpha_q\, \alpha_1^{r_1} \cdots \alpha_q^{r_q}(\zeta_j(f^1_c, \cdots, f^q_c))$$

$$\cdot (\alpha_1, \cdots, \alpha_q) = (\Omega', Q'(f^1)^{r_1} \cdots Q'(f^q)^{r_q}\Omega'), \quad (11.9)$$

and it is possible to choose $(c_j)_{j\in N}$ satisfying (11.5)

and such that

$$\lim_{j\to\infty} \int_{-\infty}^{\infty} d\alpha_1 \cdots \int_{-\infty}^{\infty} d\alpha_q\, \alpha_1^{r_1} \cdots \alpha_q^{r_q} (\zeta_j(f_{cj}^1, \cdots, f_{cj}^q)) \cdot (\alpha_1, \cdots, \alpha_q) = (\Omega', \bar{Q}'(f^1)^{r_1} \cdots \bar{Q}'(f^q)^{r_q}\Omega'), \quad (11.10)$$

i.e., the moments of $\zeta_j(f_{cj}^1, \cdots, f_{cj}^q)$ have limits which are, by the spectral theorem, the moments of the measure $\varphi \to (\Omega', \varphi(\bar{Q}'(f^1), \cdots, \bar{Q}'(f^q)\Omega'))$. By our assumption that ρ is analytic this last measure is completely determined by its moments.[17] Proposition B follows then by application of Lemma A3 (the "second limit theorem" of statistics, see Appendix).

The interpretation of (11.6) is easiest when $\mathfrak{h}'$ has a finite number d of dimensions. Let then $(\Omega_i')_{1\le i\le d}$ be an orthonormal basis of $\mathfrak{h}'$ formed by eigenvectors of all the $Q'(f)$, then (11.6) says that, *in the limit of large j one may decompose Λ_j' into d large disjoint regions of volumes $(\Omega', \Omega_i')^2 V_j$ where the correlations between the points in X_j are given by the measures μ_j on $\mathfrak{C}$ such that*

$$\mu_j(f) = (\Omega_i', \bar{Q}'(f)\Omega_i'). \quad (11.11)$$

In particular, for $q = 1$, $f^1 \in \mathfrak{C}$, one sees that the coarse-grained density $(f_{cj}^1)_{X_j}$ will take essentially only d values, which are the densities corresponding to $\mu_1, \cdots, \mu_d$. In other words, if $\mathfrak{h}'$ has d dimensions, a physical system with correlation given by μ will appear as a superposition of d different phases. This is true at least if d is finite. If d is infinite the situation is somewhat less clear. Notice that we expect $d = \infty$ to arise physically from the various orientations of a crystal lattice in treating a physical system of particles with central interactions in crystal phase. This is however an accidental degeneracy. In general one expects d to be finite. A tentative explanation of this is the following. One expects that to the decomposition $\mu = \sum_{i=1}^{d} (\Omega', \Omega_i')^2 \mu_i$ corresponds a similar decomposition of the entropy (i.e., that boundary effects between different phases contribute negligibly to the entropy). If one could forget that not every correlation functional is analytic, one would then obtain that $s(\rho)$ is *linear* in ρ on its convex set of definition. As we have seen in Sec. 10, in statistical mechanics ρ is typically solution of an extremum problem [there, to maximize $s(\rho) - \beta\rho(A)$] for a function which we expect to be linear on a convex set, and therefore "in general" $d = 1$. For other ensembles than the grand canonical, one expects d to be small.

[17] See J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, New York, 1943), p. 21, Theorem 1.12.

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APPENDIX

Lemma A1: Let F be a real function of ν arguments $m^i \in N^*$, $1 \le i \le \nu$, such that for $i = 1, \cdots, \nu$:

$$F(m^1, \cdots, m_1^i + m_2^i, \cdots, m^\nu) \ge F(m^1, \cdots, m_1^i, \cdots, m^\nu) + F(m^1, \cdots, m_2^i, \cdots, m^\nu). \quad (A1)$$

If $\sup_m (\prod_{i=1}^{\nu} m^i)^{-1} F(m)$ exists in R, the limit of $(\prod_{i=1}^{\nu} m^i)^{-1} F(m)$ when $m^1, m^2, \cdots, m^\nu$ tend to infinity exists and is equal to

$$\sup_m \left(\prod_{i=1}^{\nu} m^i\right)^{-1} F(m).$$

This is an easy generalization of Exercise 98 in the first part of the first volume of the exercise book of Pólya and Szegö.[18]

Lemma A2: Let $\alpha \in R_+^*$. If the real function f, defined in an open interval I of R, is increasing and satisfies the inequality

$$f[(\lambda' + \lambda'')/2] \ge (1 - \alpha)f(\lambda') = \alpha f(\lambda'') \quad (A2)$$

for all $\lambda', \lambda'' \in I$ such that $\lambda' < \lambda''$, then f is continuous in I.

Let $\lambda \in I$ and $\epsilon \in R_+^*$. We define

$$f_-(\lambda) = \lim_{\epsilon\to 0} f(\lambda - \epsilon), \quad f_+(\lambda) = \lim_{\epsilon\to 0} f(\lambda + \epsilon). \quad (A3)$$

Taking $\lambda' = \lambda - 2\epsilon$, $\lambda'' = \lambda + \epsilon$ we obtain from (A2)

$$f_-(\lambda) \ge (1 - \alpha)f_-(\lambda) + \alpha f_+(\lambda); \quad (A4)$$

hence $f_-(\lambda) \ge f_+(\lambda)$.

Lemma A3: Let the measures $\zeta_j \ge 0$ on $R^q (q \in N^*)$ be defined for all $j \in N$ and have moments of all orders. We assume that there exists a measure $\zeta \ge 0$ on R^q such that (using a functional notation for measures)

$$\lim_{j\to\infty} \int_{-\infty}^{\infty} d\alpha_1 \cdots \int_{-\infty}^{\infty} d\alpha_q\, \alpha_1^{r_1} \cdots \alpha_q^{r_q} \zeta_j(\alpha) = \int_{-\infty}^{\infty} d\alpha_1 \cdots \int_{-\infty}^{\infty} d\alpha_q\, \alpha_1^{r_1} \cdots \alpha_q^{r_q} \zeta(\alpha) \quad (A5)$$

[18] G. Pólya and G. Szegö, *Aufgaben und Lehrsätze aus der Analysis* (Springer-Verlag, Berlin, 1954), Vol. 1, 2nd ed.

for all $r_1, \cdots, r_q \in N$. Then, if ζ is determined by its moments, we have for any real continuous function φ with compact support in R^q

$$\lim_{j\to\infty} \int_{-\infty}^{\infty} d\alpha_1 \cdots \int_{-\infty}^{\infty} d\alpha_q \, \varphi(\alpha)\zeta_j(\alpha) = \int_{-\infty}^{\infty} d\alpha_1 \cdots \int_{-\infty}^{\infty} d\alpha_q \, \varphi(\alpha)\zeta(\alpha). \quad \text{(A6)}$$

This is simply the "second limit theorem" of statistics, which is however usually proved for $q = 1$. The one-dimensional proof given in Ref. 19, pp. 127–128, may however easily be extended to $q > 1$.[20]

[19] S. S. Wilks, *Mathematical Statistics* (John Wiley & Sons, Inc., New York, 1962).

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The Structure of Space and the Formalism of Relativistic Quantum Theory. II

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A purely group theoretical treatment of interactions of relativistic particles is shown to be possible in the connection of a finite geometry of space-time. The S operators are constructed by means of the reductions of the irreducible unitary representations of the relativity group of space-time. The dependence of the S-matrix elements on the momenta is still nontrivial, since there is a nontrivial distribution of observable momenta in a finite geometry. The Feynman graphs are easily evaluated by a simple computational technique involving five rules. The coupling schemes corresponding to nuclear electromagnetic, and weak forces in finite geometry are considered.

I. GENERAL STRUCTURE OF THE FOCK–HILBERT SPACE

CONSIDER the irreducible manifolds $H(M, S, Q)$ of the Dieudonné group $\mathfrak{D}'$ (cf. Paper I of this series).[1] Let us denote the labels (M, S, Q) by a single index λ which then represents the particle species. A given manifold H_λ contains all the single-particle states of a particle of the species λ, and this space carries an irreducible unitary representation U_λ of the Dieudonné group $\mathfrak{D}'$. The space $H_{\bar\lambda}$ carrying the representation U_λ^* contains the single-particle states of the antiparticle $\bar\lambda$.

For any boson or fermion (particle or antiparticle) species λ we introduce a larger space K_λ by

$$K_\lambda = H_0(\lambda) \oplus_{n=1}^{\infty} S(\otimes^n H_\lambda) \quad \text{if } \lambda \text{ is a boson species,}$$
$$K_\lambda = H_0(\lambda) \oplus_{n=1}^{h(\lambda)} A(\otimes^n H_\lambda) \quad \text{if } \lambda \text{ is a fermion species.} \quad \text{(1)}$$

Here S and A are the symmetry and the antisymmetry operators, respectively, in the n-fold tensor spaces $\otimes^n H_\lambda$ in question (for their definition, see Greub[2]). The space $H_0(\lambda)$ is a one-dimensional linear space carrying the identity representation of $\mathfrak{D}'$.

Notice that the series of K_λ in (1) contains in the fermion case only a finite number of terms. This is a consequence of the finitness of the dimensionality of the space H_λ in finite geometry, and the number $h(\lambda)$ is exactly the number of the dimensions of H_λ (cf. Greub[2]):

$$h(\lambda) = \dim H_\lambda. \quad \text{(2)}$$

Consider the spaces

$$K = \otimes_\lambda K_\lambda, \quad H = \oplus_\lambda H_\lambda, \quad \lambda \in \Omega, \quad \text{(3)}$$

where Ω is a finite set of particle species. The space K is the general Fock–Hilbert space[3] which contains the states of all the systems composed of the particles $\lambda \in \Omega$, and in which the interactions of these particles are to be described. The space H is the total single-particle space of all the particles $\lambda \in \Omega$.

[1] Y. Ahmavaara, J. Math. Phys. 5, 87 (1964).

[2] W. Greub, *Linear Algebra* (Springer-Verlag, Berlin, 1963).

[3] V. Fock, Z. Physik 75, 622 (1932).

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[2] W. Greub, *Linear Algebra* (Springer-Verlag, Berlin, 1963).

[3] V. Fock, Z. Physik 75, 622 (1932).

Introducing a projection operator P which symmetrizes with respect to identical bosons, and antisymmetrizes with respect to identical fermions, one can evaluate K in terms of the single-particle space H:

$$K = K(1) \oplus H \oplus P(H \otimes H) \oplus P(H \otimes H \otimes H) \oplus \cdots . \tag{4}$$

Here

$$P(\overset{n}{\otimes} H)$$

is composed of all the n-particle states of the particles $\lambda \in \Omega$, and the space

$$K(1) = \bigotimes_{\lambda} H_0(\lambda)$$

contains only the mathematical vacuum state Φ_0.

We introduce complete orthonormal bases in the spaces H_λ and K_λ, and denote them, respectively, as follows:

$$\begin{aligned} H_\lambda &: \{\Phi_j(\lambda); j = 1, 2, \cdots, h(\lambda)\}, \\ K_\lambda &: \{\xi_{n(\lambda)}; n(\lambda) \in \Delta_\lambda\}. \end{aligned} \tag{5}$$

Here Δ_λ is the set of all the sequences

$$n(\lambda) = (n_1(\lambda), n_2(\lambda), \cdots, n_{h(\lambda)}(\lambda)), \quad n_j(\lambda) \geq 0,$$

where the integer $n_j(\lambda)$ is the number of the particles of the single-particle state $\Phi_j(\lambda)$ present in the state $\xi_{n(\lambda)}$. The number

$$\sum_{j=1}^{h(\lambda)} n_j(\lambda)$$

thus gives the total number of particles present in the state $\xi_{n(\lambda)}$. The set Δ_λ becomes a semigroup by the definition of addition of sequences:

$$n(\lambda) + n'(\lambda) = (n_1(\lambda) + n_1'(\lambda), n_2(\lambda) + n_2'(\lambda), \cdots). \tag{6}$$

In particular, we define the sequences

$$\begin{aligned} \delta_j(\lambda) &= (0, \cdots, 0, 1, 0, \cdots, 0) \\ 0(\lambda) &= (0, 0, \cdots, 0), \end{aligned} \tag{7}$$

and

where 1 is in the jth place in the sequence $\delta_j(\lambda)$, while $0(\lambda)$ is the sequence of zeros.

After these definitions we have

$$\begin{aligned} \xi_{0(\lambda)} &\in H_0(\lambda), \\ \xi_{\delta_j(\lambda)} &= \Phi_j(\lambda) \in H_\lambda, \\ \xi_{\delta_j(\lambda)+\delta_k(\lambda)} &\sim P(\Phi_j(\lambda) \cdot \Phi_k(\lambda)) \in P(\overset{2}{\otimes} H_\lambda), \\ \xi_{n(\lambda)} &\sim P(\prod_j \Phi_j(\lambda)) \in P(\overset{n}{\otimes} H_\lambda) \quad \text{if} \quad \sum_{j=1}^{h(\lambda)} n_j(\lambda) = n. \end{aligned} \tag{8}$$

Here P is A for a fermionic λ, and S for a bosonic λ.

A complete basis of the total Fock–Hilbert space K is now given by the tensorial product states of the form

$$\Phi_{n(\lambda), m(\lambda'), \cdots} = \xi_{n(\lambda)} \xi_{m(\lambda')} \cdots \tag{9}$$

Evidently, the state (9) belongs to the n-particle space

$$P(\overset{n}{\otimes} H) \quad \text{if} \quad \sum_{j=1}^{h(\lambda)} n_j(\lambda) + \sum_{k=1}^{h(\lambda')} m_k(\lambda') + \cdots = n.$$

In particular, the normalized mathematical vacuum state is represented by

$$\Phi_{0,0,\cdots,0} = \prod_{\lambda} \xi_{0(\lambda)}. \tag{10}$$

A complete set of operators in the space K is obtained by introducing the set of the creation and the annihilation operators

$$\{a_j^\dagger(\lambda), a_j(\lambda); j = 1, 2, \cdots, h(\lambda); \lambda \in \Omega\}$$

by the defining formulas

$$\begin{aligned} a_j^\dagger(\lambda)\Phi_{n(\lambda),\cdots} &= C_\lambda(j, n)\Phi_{n(\lambda)+\delta_j(\lambda),\cdots}, \\ a_j(\lambda)\Phi_{n(\lambda),\cdots} &= \begin{cases} C_\lambda(j, n - \delta_j)^* \Phi_{n(\lambda)-\delta_j(\lambda),\cdots} & \\ \qquad \text{if} \quad n_j(\lambda) > 0 & \\ 0 \qquad \text{if} \quad n_j(\lambda) = 0. & \end{cases} \end{aligned} \tag{11}$$

Here

$$C(j, n) = \begin{cases} (n_j + 1)^{\frac{1}{2}} \quad \text{for a boson } \lambda \\ \delta_{0, n_j(\lambda)} (-1)^{n_1(\lambda) + \cdots + n_j(\lambda)} \\ \qquad \text{for a fermion } \lambda. \end{cases} \tag{12}$$

Evidently, the operators $a_j^\dagger(\lambda)$ and $a_j(\lambda)$ of a fermonic λ are proper, bounded operators of K, while those of a bosonic λ are proper but nonbounded. This is due to the fact that the bosonic occupation numbers have no upper limit.

The transformation properties of the single-particle states of a particle and its antiparticle imply those of the respective creation and the annihilation operators in the following way:

$$\begin{aligned} &\text{the } a_j^\dagger(\lambda) \text{ carry } U_\lambda, \\ &\text{the } a_j(\lambda) \text{ carry } U_\lambda^*, \\ &\text{the } a_j^\dagger(\bar{\lambda}) \text{ carry } U_\lambda^*, \\ &\text{the } a_j(\bar{\lambda}) \text{ carry } U_\lambda. \end{aligned} \tag{13}$$

II. THE CONSTRUCTION OF THE SCATTERING OPERATOR

Mathematically speaking, a "scattering operator" S is a unitary operator of K, composed of the crea-

tion and the annihilation operators, and invariant with respect to the relativity group. Physically, a given S describes interaction between the particle species whose creation and annihilation operators are involved in this particular S.

Let us see, by the way of a simple example, how a purely group theoretical construction leads to a unique S operator for the description of an interaction between given particle species. The following construction works well only in finite geometry—it should be kept in mind that in a finite geometry the observable states of momentum have a nontrivial distribution of geometrical origin (cf. Paper I, Sec. V).

Consider two fermion species a and b, and a boson species ω, such that $\bar{a} \neq a$, $\bar{b} \neq b$, and $\bar{\omega} \neq \omega$. Neglecting for a while the contributions of the antiparticles to the interaction between a, b, and ω the Fock–Hilbert space of interaction of these particle species is simply

$$K = K_a \otimes K_b \otimes K_\omega. \tag{14}$$

For the construction of an S operator one has at his disposal the following creation and annihilation operators with the respective irreducible unitary representations of the relativity group according to which they transform:

$$\begin{aligned} &\text{the } a_i^\dagger : U_a, \quad \text{the } a_i : U_a^*, \\ &\text{the } b_k^\dagger : U_b, \quad \text{the } b_k : U_b^*, \\ &\text{the } \omega_l^\dagger : U_\omega, \quad \text{the } \omega_l : U_\omega^*. \end{aligned} \tag{15}$$

Let us assume that the reduction formula

$$U_a^* \otimes U_b \sim U_\omega^* \oplus \cdots \tag{16}$$

holds true. It then follows from (15) and (16) that the operator

$$\sum_i \sum_k g(jkl) a_i b_k^\dagger = c_l,$$

where the $g(jkl)$ are the reduction coefficients, transforms with respect to the relativity group $\mathfrak{D}'$ just like the annihilation operator ω_l. Accordingly, the operator

$$\sum_i \sum_k \sum_l g(jkl) a_i b_k^\dagger \omega_l^\dagger = \vartheta \tag{17}$$

is invariant with respect to the transformations of the relativity group.

The "vertex operator" ϑ of (17) gives rise to a fundamental process, or a "coupling" $a \rightarrow b + \omega$ between the particle species a, b, and ω.

By complex conjugation (16) gives at once another reduction formula holding good simultaneously with (16), viz.,

$$U_a \otimes U_b^* \sim U_\omega \oplus \cdots . \tag{18}$$

This gives the vertex operator $\vartheta^\dagger$ and the inverted coupling $a \leftarrow b + \omega$.

From the two vertex operators ϑ and $\vartheta^\dagger$ one can already construct a scattering operator, the simplest possible one. To this end one has to combine first the vertex operators to a Hermitian one:

$$\theta = c\vartheta + c^*\vartheta^\dagger. \tag{19}$$

Here c is a complex "coupling constant." This Hermitian gives the scattering operator

$$S = e^{i\theta} = 1 + i\theta + (2!)^{-1} i^2 \theta^2 + (3!)^{-1} i^3 \theta^3 + \cdots . \tag{20}$$

This scattering operator describes all those processes of interaction between the species a, b, and ω, which are due to the coupling scheme $a \leftrightarrow b + \omega$, and to this scheme only.

Note: One may ask why it is just in a finite geometry that one can apply the purely group theoretical construction of S operator illustrated above. In fact, the reduction formulas of the above kind can be written down even for the irreducible unitary representations of the relativity group (the inhomogeneous Lorentz group) of continuous space–time.

However, the group theoretical method cannot be applied in the case of continuous topology, since it would in continuous topology lead to S-matrix elements whose dependence on the momenta of the particles were of a trivial kind. Indeed, the relativistic invariance implies, as far as the momenta are concerned, just the law of conservation of momentum, and nothing more. Thus the complicated dependence of interactions on the momenta, apparent in the experimental results, could not be thought to be explained by a purely group theoretical formalism in continuous topology.

In continuous topology of space–time (in the quantum field approach), the dilemma of the momentum dependence of interactions is attacked about in the following way.[4] One decomposes the irreducible unitary representations U of the relativity group to a direct product

$$U \sim T \otimes M, \tag{21}$$

where M is a spinor representation of the homogeneous Lorentz group.[5] Then one applies the reduction formulas for the spinor representations only. This gives Lorentz-invariant vertex operators, say,

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[4] What follows is the consideration of a simple special case. For a more complete analysis of the group structure of quantum field theory see Y. Ahmavaara, Ann. Acad. Sci. Fennicae Ser. AVI, No. 106 (1962).

[5] In general, quantum field theory implies only the assumption that there is a homomorphism $T \otimes M \simeq U \oplus U^*$, see Ref. 4, p. 18.

$\vartheta(p_a, p_b, p_\omega)$, which still depend on the momenta of the particles in question.

Thus only a *partial reduction*, viz., a reduction of the part M of the total representation U, is applied in quantum field theory. This is the "postulate of the partial reduction" which is implied in all quantum field theories (cf., Ahmavaara Ref. 4, pp. 17–18).

The rest of the construction of S operator is performed, in quantum field theory, by using another technique of constructing invariants, viz., the method *invariant integration* (for a closer analysis of the combination of the two techniques in current quantum field theories see Ahmavaara, Ref. 4). By Lorentz-invariant integration over the momentum space one obtains the final vertex operators which are invariant with respect to the translations of space–time too. The integrals involve, however, arbitrary Lorentz-invariant functions. For the determination of these functions one can try to apply either (1) the classical dynamical Hamilton–Lagrange formalism (the historical quantum field theory which is inconsistent mathematically), or (2) the condition of "microcausality" (the axiomatic quantum field theory of Haag, Lehmann, Wightman, *et al.*[6]), or (3) the condition of "analyticity" (the pure S-matrix theory of Chew *et al.*[7]).

In a finite geometry the group theoretical reduction method can be used in its full capacity, and not only "partially." It involves no arbitrary functions. The dependence of the S-matrix elements on the momenta will not be a trivial one. This is due to the fact that there is in this case a nontrivial distribution of the observable states of momentum. This distribution is a consequence of the condition of "Euclidicity" which must be imposed on the observable 4-momenta in a finite geometry (cf. Paper I, Sec. V).

The group theoretical method of constructing the S operators thus implies the idea that the momentum dependence of the interactions of relativistic particles cannot be explained, in general, (1) by a variational principle, nor (2) by microcausality, nor (3) by analyticity, but by the geometrical relations of Euclidicity characteristic to a finite geometry of space–time.

III. THE CALCULATION OF THE FEYNMAN GRAPHS

Let us see how the Feynman graphs are evaluated by the group theoretical method. The graphs associated with the scattering operator (20) may serve as examples.

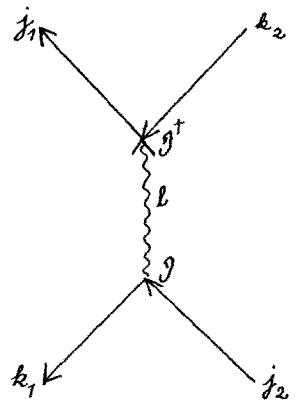

FIG. 1.

Consider, for instance, the contribution of the second-order graph of Fig. 1 to the respective matrix element of θ^2. Using the Dirac notation for states, by writing

$$\Phi_j(a) = |j\rangle, \qquad \Phi_k(b) = |k\rangle, \quad \text{etc.},$$

the matrix element in question is $\langle j_1 k_1| \ \theta^2 \ |j_2 k_2\rangle$.

As indicated in Fig. 1 the lower vertex of the graph is described by the operator ϑ, and the upper vertex by the operator $\vartheta^\dagger$, the whole graph being described by the product $\vartheta^\dagger\vartheta$. The contribution to the matrix element is calculated by using the following simple rules: (1) Write down the relevant product of the reduction coefficients, provided by the correct subscripts read from the graph, $g^*(j_1 k_2 l)g(j_2 k_1 l)$. (2) Sum over the index l of the virtual boson states. (3) Multiply by the relevant coupling constants c and c^*. (4) Check whether there appear two (or more) simultaneous identical fermions in the course of the process—they must be excluded, of course; in the present case, the contribution is $\neq 0$ only if $k_1 \neq k_2$; this gives rise to the Kronecker factor $1 - \delta_{k_1 k_2}$ in the matrix element. (5) Check whether there appear two (or more) simultaneous identical bosons in the course of the process; this is not the case now, since there is only one virtual boson. The final result thus is

$$\langle j_1 k_1| \ \theta^2 \ |j_2 k_2\rangle = cc^*(1 - \delta_{k_1 k_2}) \times \sum_l g^*(j_1 k_2 l)g(j_2 k_1 l). \qquad (22)$$

As an example of a graph where also the rule (5) has application, consider the fourth-order "crossing graph" of Fig. 2. This graph is described by the product $\vartheta^\dagger\vartheta^\dagger\vartheta\vartheta$ of the vertex operators. The same computational steps as before give now the following:

[6] L. Klein, *The Dispersion Relations and the Abstract Approach to Field Theory* (Gordon and Breach, Inc., New York, 1961).

[7] G. Chew, *S-Matrix Theory of Strong Interactions* (W. A. Benjamin, Inc., New York, 1962).

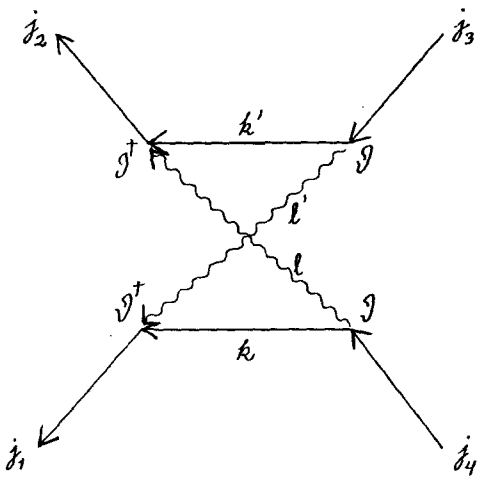

FIG. 2.

(1) The product of the relevant reduction coefficients is

$$g^*(j_1kl')g^*(j_2k'l)g(j_3k'l')g(j_4kl).$$

(2) The summation over the virtual states gives

$$\sum_k \sum_{k'} \sum_l \sum_{l'}.$$

(3) The relevant product of the coupling coefficients is $ccc^*c^* = |c|^4$. (4) Initially, there are two fermions j_3 and j_4, and finally two fermions j_1 and j_2—there must be $j_3 \neq j_4$ and $j_1 \neq j_2$ which is indicated by the respective coefficients $1 - \delta_{j_1j_2}$ and $1 - \delta_{j_3j_4}$ in the matrix element. (5) Between the second and the third vertex processes there are two bosons l and l' simultaneously present; in the case that $l' = l$ the creation and the annihilation of the second boson give together a coefficient $\sqrt{2}\sqrt{2} = 2$ to the respective matrix element. Accordingly, the total result can be written

$$\begin{aligned}\langle j_1j_2|\ \theta^4\ |j_3j_4\rangle &= |c|^4\,(1-\delta_{j_1j_2})(1-\delta_{j_3j_4})\\ &\times \sum_{k'\neq k}\sum_k \{\sum_{l'\neq l}\sum_l g^*(j_1kl')g^*(j_2k'l)g(j_3k'l')g(j_4kl)\\ &+ 2\sum_l g^*(j_1kl)g^*(j_2k'l)g(j_3k'l)g(j_4kl)\}. \qquad (23)\end{aligned}$$

Using the rules (1)–(5) one can easily evaluate any Feynman graph connected with the simple scattering operator (20) of our example and, in fact, any graph of any scattering operator constructed by the group theoretical method. In general the rules (1)–(5) give only the absolute value of the matrix element in question. The sign must be determined separately by the formula (12).

IV. THE DESCRIPTION OF THE NUCLEAR, ELECTROMAGNETIC, AND WEAK INTERACTIONS

The example of 3-particle coupling considered above was oversimplified: for instance, the contributions of the antiparticles were neglected. Let us now see what kinds of couplings are needed for the description of realistic physical forces in finite geometry.

Let us begin by the two fermion species a and b, and the boson species ω, considered above. At first we again make the assumption $\bar{a} \neq a$, $\bar{b} \neq b$, and $\bar{\omega} \neq \omega$, as well as $a \neq b$. Taking now the antiparticles too into account the Fock–Hilbert space of the complete set $(a, b, \omega, \bar{a}, \bar{b}, \bar{\omega})$ of particle and antiparticle species is given by

$$K = K_a \otimes K_{\bar{a}} \otimes K_b \otimes K_{\bar{b}} \otimes K_\omega \otimes K_{\bar{\omega}}. \qquad (24)$$

For the construction of the scattering operator one has now at his disposal the following six kinds of creation and annihilation operators with their respective modes of transformation:

$$\begin{aligned}&\left.\begin{matrix}\text{the } a_i^\dagger\\ \text{the } \bar{a}_i\end{matrix}\right\} : U_a \qquad \left.\begin{matrix}\text{the } a_i\\ \text{the } \bar{a}_i^\dagger\end{matrix}\right\} : U_a^*\\ &\left.\begin{matrix}\text{the } b_k^\dagger\\ \text{the } \bar{b}_k\end{matrix}\right\} : U_b \qquad \left.\begin{matrix}\text{the } b_k\\ \text{the } \bar{b}_k^\dagger\end{matrix}\right\} : U_b^* \qquad (25)\\ &\left.\begin{matrix}\text{the } \omega_l^\dagger\\ \text{the } \bar{\omega}_l\end{matrix}\right\} : U_\omega \qquad \left.\begin{matrix}\text{the } \omega_l\\ \text{the } \bar{\omega}_l^\dagger\end{matrix}\right\} : U_\omega^*.\end{aligned}$$

The reduction formula (the same as before)

$$U_a^* \otimes U_b \sim U_\omega^* \oplus \cdots \qquad (26)$$

now gives five vertex operators describing vertices where two particles are converted to one particle, viz., the following ones:

$$\begin{aligned}\vartheta_1 &= \sum_{jkl} g(jkl)a_jb_k^\dagger\omega_l^\dagger \qquad (a \to b + \omega)\\ \vartheta_2 &= \sum_{jkl} g(jkl)a_j\bar{b}_k\omega_l^\dagger \qquad (a + \bar{b} \to \omega)\\ \vartheta_3 &= \sum_{jkl} g(jkl)\bar{a}_j^\dagger\bar{b}_k\omega_l^\dagger \qquad (\bar{b} \to \bar{a} + \omega) \qquad (27)\\ \vartheta_4 &= \sum_{jkl} g(jkl)a_jb_k^\dagger\bar{\omega}_l \qquad (a + \bar{\omega} \to b)\\ \vartheta_5 &= \sum_{jkl} g(jkl)\bar{a}_j^\dagger\bar{b}_k\bar{\omega}_l \qquad (\bar{b} + \bar{\omega} \to \bar{a}).\end{aligned}$$

The complex conjugation of (26) yields still five vertex operators, viz., the adjoints of (27), and the respective time-inverted couplings. The scattering operator corresponding to the reduction (26) is now given by

$$S = e^{i\eta}, \qquad \eta = \sum_{\nu=1}^{5}(c_\nu\vartheta_\nu + c_\nu^*\vartheta_\nu^\dagger). \qquad (28)$$

If one counts fermions by a "fermion number" defined to be $+1$ for the fermionic particles and -1 for the fermionic antiparticles, then the couplings involved in (28) can all be represented by the two couplings

$$a \leftrightarrow b + \omega \quad \text{and} \quad b \leftrightarrow a + \bar{\omega} \tag{29}$$

plus the law of conservation of fermion number.

The nuclear force between protons and neutrons is generally assumed to be due to the couplings $p \leftrightarrow n + \pi^+$ and $n \leftrightarrow p + \pi^-$ (there being $\pi^- = \bar{\pi}^+$), and to the couplings obtained from these by the law of conservation of baryon (=heavy fermion) number. Such a coupling scheme is an example of (29). Accordingly, a reduction formula of the type (26) and the scattering operator defined by (27)–(28) give the theory of this nuclear force in a finite geometry. Other examples of this coupling are among those which are suggested to hold for strong interactions of the "strange particles", for instance, the Λ couplings:

$$n \leftrightarrow \Lambda + K^0 \quad \text{and} \quad \Lambda \leftrightarrow n + \bar{K}^0$$
$$p \leftrightarrow \Lambda + K^+ \quad \text{and} \quad \Lambda \leftrightarrow p + K^-$$
$$\Sigma^{+-} \leftrightarrow \Lambda + \pi^{+-} \quad \text{and} \quad \Lambda \leftrightarrow \Sigma^{+-} + \pi^{-+}.$$

In particular, it can happen that $\bar{\omega} = \omega$ or, what is the same, that there is an equivalence

$$U_\omega \sim U_\omega^*. \tag{30}$$

Of course, the Fock–Hilbert space K of (24) now must be reduced to a fivefold direct product only, the factor K_ω being left out. The vertex operators are again those of (27), except that in ϑ_4 and in ϑ_5 the operators $\bar{\omega}_l$ must be replaced by the ω_l. The coupling scheme is now given by

$$a \leftrightarrow b + \omega \quad \text{and} \quad b \leftrightarrow a + \omega \tag{31}$$

plus the law of conservation of fermion number. This kind of coupling is suggested to hold, for instance, between the neutral Λ and Σ particles:

$$\Sigma^0 \leftrightarrow \Lambda + \pi^0 \quad \text{and} \quad \Lambda \leftrightarrow \Sigma^0 + \pi^0.$$

Let us now make the restriction that $a = b$. From the corresponding reduction formula

$$U_a^* \otimes U_a \sim U_\omega^* \oplus \cdots \tag{32}$$

and from its complex conjugate it follows that $U_\omega \sim U_\omega^*$ or $\bar{\omega} = \omega$. Accordingly, $a = b$ imples $\bar{\omega} = \omega$.

The Fock–Hilbert space of interaction of a, $\bar{a}$, and ω of course reduces to the threefold direct product of K_a, $K_{\bar{a}}$, and K_ω. The number of vertex operators is reduced from 10 to 6. The formula (32) gives

$$\begin{aligned}
\vartheta_1' &= \tfrac{1}{2} \sum_{jkl} g(jkl)(a_j a_k^\dagger + a_k^\dagger a_j)\omega_l \qquad (a \to a + \omega) \\
\vartheta_2' &= \sum_{jkl} g(jkl) a_j \bar{a}_k \omega_l^\dagger \qquad (a + \bar{a} \to \omega) \\
\vartheta_3' &= \tfrac{1}{2} \sum_{jkl} g(jkl)(\bar{a}_j^\dagger \bar{a}_k + \bar{a}_k \bar{a}_j^\dagger)\omega_l^\dagger \qquad (\bar{a} \to \bar{a} + \omega).
\end{aligned} \tag{33}$$

A symmetrization with respect to the order of a_j and $a_k^\dagger$, and of $\bar{a}_j$ and $\bar{a}_k^\dagger$ is taken into account. The complex conjugate formula gives the adjoint vertex operators. The S operator is thus given by

$$S = e^{i\eta'}, \qquad \eta' = \sum_{\nu=1}^{3} (c_\nu' \vartheta_\nu' + c_\nu'^* \vartheta_\nu'^*). \tag{34}$$

The couplings involved in (33)–(34) are represented by

$$a \leftrightarrow a + \omega \tag{35}$$

plus the law of conservation of fermion number. Physical examples of this kind of coupling scheme are the electromagnetic couplings $e \leftrightarrow e + \gamma$ (between electrons and photons), and $p \leftrightarrow p + \gamma$ (between protons and photons), and the nuclear couplings $n \leftrightarrow n + \pi^0$ (between neutrons and neutral pions), and $p \leftrightarrow p + \pi^0$ (between protons and neutral pions), there being $\bar{\gamma} = \gamma$ and $\bar{\pi}^0 = \pi^0$. Accordingly, the electromagnetic forces and the nuclear forces between neutrons themselves and protons themselves must in finite geometry be described by reduction formula of the type (32), and by the respective S operator (34).

Let us now consider four fermion species a, b, c, and d, and a reduction formula of the type

$$U_a^* \otimes U_b \sim (U_c^* \otimes U_d) \oplus \cdots . \tag{36}$$

This corresponds to the simultaneous validity of the following reductions of the direct product representations to their irreducible components:

$$\begin{aligned}
&U_c^* \otimes U_d \sim \bigoplus_\lambda U_\lambda, && \lambda \in \Omega_0, \\
&U_a^* \otimes U_b \sim (\bigoplus_\lambda U_\lambda) \oplus \cdots, && \lambda \in \Omega_0.
\end{aligned} \tag{37}$$

Notice that here it is not sufficient that the decompositions of $U_a^* \otimes U_b$ and $U_c^* \otimes U_d$ have just a common term say, U_ω, in their decompositions but it is required that *all* the irreducible components of $U_c^* \otimes U_d$ are among the irreducible components of $U_a^* \otimes U_b$.

The Fock–Hilbert space of interactions of the four particle and four antiparticle species is, of course, an eightfold direct product space. It follows

from the reduction formula (36) that the operators

$$\sum_{ik} h(jkln)a_i b_k^\dagger = A_{ln},$$

where the $h(jkln)$ are the reduction coefficients, transform just like the products $c_l d_n^\dagger$. Accordingly, the operator

$$\sum_{jkln} h(jkln)a_j b_k^\dagger c_l^\dagger d_n = \chi \tag{38}$$

is invariant.

Other vertex operators are obtained from (38) by replacing creation and annihilation operators by antiparticle annihilation and creation operators, respectively, and by taking the adjoints. The scattering operator will be given by

$$S = e^{iX}, \qquad X = \sum_\nu (f_\nu \chi_\nu + f_\nu^* \chi_\nu^\dagger). \tag{39}$$

This scattering operator, and the underlying reduction formula (36), correspond to a direct four-particle coupling represented by

$$a + d \leftrightarrow b + c \tag{40}$$

plus the couplings obtained from this by the law of conservation of fermion number. Physical examples of this kind of couplings are the couplings describing the weak interactions. Accordingly, one must assume that the weak interactions are described by reductions of the type (36), and by respective S operators (40), in finite geometry.

Evidently, one can continue the process of constructing coupling schemes to higher orders of (even weaker?) direct n-particle couplings. The present physics has not found their traces in experiments, however, with the exception of one more coupling describing the gravitational interaction. If the spin of the graviton is 2, the gravitational interaction could be described for instance by a direct five-particle coupling between the graviton and four fermions of spin $\frac{1}{2}$. Such a coupling has not been studied in physics so far.

Note 1: In conventional quantum theory connected with continuous topology of space–time one has been accustomed to describe the strength of interaction by the magnitude of the respective coupling constants. It follows that a quantitative theory has been possible only for the electromagnetic and for the weak interactions. In the case of strong interactions, one must substitute coupling constants so large that the exponential series of S operator diverges, each of the successive terms giving contributions larger than the previous terms.

In finite geometry no difficulty of this kind seems necessary. One must remind that the experimental measure of the strengthness of interaction is the inverted lifetime or, what is the same, the so-called transition rate. This depends not only on the magnitude of the S-matrix element in question but also on the number of the final states per unit energy interval. In finite geometry, there is a nontrivial distribution of the observable states of momentum (cf. Paper I, Sec. V) which implies also a nontrivial spectrum of energy for each mass value.

The energy spectrum depends on the mass of the particle in a sensitive way. As an over-all rule, however, one can state that the density of states per unit energy tends to grow with increasing rest mass (for the masses $m \neq 0$). Accordingly, interactions between heavy particles tend to be stronger than those between light particles in finite geometry. If the energy spectrum is dominating for the strengthness of interactions in finite geometry, then even small coupling constants may lead to strong interactions, and a quantitative theory of strong interactions can be based on an exponential S operator.

There is another effect due to the density of states in finite geometry. Evidently, the three-particle interactions are of observable magnitude for those particle species a, b, and ω, whose irreducible state manifolds H_a, H_b, and H_ω contain a very large number of observable states of momentum. Accordingly, they are bound to occur between particles representing the peaks of the mass spectrum. On the other hand, the four-particle interactions (or, *a fortiori*, any n-particle interactions for $n \geq 4$) based on the reduction formula (36) necessarily involve, as is indicated by (37), a large number of "intermediate" particle species λ. These species λ are associated with mass values which probably are rather randomly distributed, and are by no means just the peaks of the mass spectrum. Accordingly, the density of states connected with a four-particle coupling must be assumed very low in comparison with the observable three-particle interactions. Thus one could qualitatively understand why the four-particle couplings already describe very weak interactions. Of course, this is an unproved suggestion.

Note 2: Another remark to be made here concerns the consistency of the present formalism. As soon as antiparticles too are involved in the Fock–Hilbert space this space has, evidently, a degenerated vacuum state. In other words, there are elements of K other than the absolute vacuum state $\Phi_{0,0,\ldots}$ which are invariant in the relativity group. Let us call these elements "relativistic vacuum states," and consider them in some detail.

Since the single-particle states of a particle and

its antiparticle transform contravariantly with respect to one another, there is a relativistic vacuum state for every pair of particle–antiparticle species involved in the interaction. In the K space (24) of our example there are thus, in general, three relativistic vacuum states of this kind, viz.

$$\begin{aligned}\sum_i \Phi_i(a)\Phi_i(\bar{a}) &= \Phi_0(a\bar{a}),\\ \sum_k \Phi_k(b)\Phi_k(\bar{b}) &= \Phi_0(b\bar{b}),\\ \sum_l \Phi_l(\omega)\Phi_l(\bar{\omega}) &= \Phi_0(\omega\bar{\omega}).\end{aligned} \tag{41}$$

Let the "two-particle vacuum space" spanned by these three invariant two-particle states be denoted by $K(2)$. Evidently, $K(2) \subset P(H \otimes H)$.

Another type of relativistic vacuum states is obtained by means of a reduction formula. For instance, it follows from the reduction formula (26) of our example that the two-particle states

$$\begin{aligned}\sum_{jk} g(jkl)\Phi_j(\bar{a})\Phi_k(b) &= \Psi_l(\bar{\omega}),\\ \sum_{jk} g^*(jkl)\Phi_j(a)\Phi_k(\bar{b}) &= \Psi_l(\omega)\end{aligned} \tag{42}$$

transform like the single-particle states $\Phi_l(\bar{\omega})$ and $\Phi_l(\omega)$, respectively. Thus the three-particle states

$$\begin{aligned}\sum_{jkl} g(jkl)\Phi_j(\bar{a})\Phi_k(b)\Phi_l(\omega) &= \Phi_0(\bar{a}b\omega),\\ \sum_{jkl} g^*(jkl)\Phi_j(a)\Phi_k(\bar{b})\Phi_l(\bar{\omega}) &= \Phi_0(a\bar{b}\bar{\omega})\end{aligned} \tag{43}$$

are invariant. Let the "three-particle vacuum space" spanned by these two invariant three-particle states be denoted by $K(3)$. Evidently,

$$K(3) \subset P(H \otimes H \otimes H).$$

The basic relativistic vacuum spaces $K(2)$ and $K(3)$ generate further relativistic vacuum spaces by their direct products and direct sums:

$$\begin{aligned}K(4) &= K(2) \otimes K(2) \subset P(\overset{4}{\otimes} H),\\ K(5) &= K(2) \otimes K(3) \subset P(\overset{5}{\otimes} H),\\ K(6) &= (K(2) \otimes K(2) \otimes K(2))\\ &\quad \oplus (K(3) \otimes K(3)) \subset P(\overset{6}{\otimes} H), \quad \text{etc.}\end{aligned} \tag{44}$$

The total relativistic vacuum is given by the direct sum

$$K_0 = K(2) \oplus K(3) \oplus K(4) \oplus \cdots . \tag{45}$$

The existence of a degenerated vacuum implies, however, no inconsistency in the physical interpretation of quantum states. This is due to the facts that (1) no combination of the observable states is a vacuum state, and (2) any vacuum state can not either be reached by a Lorentz transformation from given observable states.

On the other hand, the existence of relativistic vacuum states implies no inconsistency in the mathematical formalism either, since there is still only one state upon which the creation and the annihilation operators operate as on the "vacuum."

Exponential Ensemble for Random Matrices*

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Using the ideas of information theory, it is pointed out that the Gaussian ensemble for random Hermitian matrices can be characterized as the "most random" ensemble of these matrices. Pursuing the same characterization for positive matrices, we are led in a natural way to the definition of the exponential ensemble. Transforming to a representation of eigenvectors and eigenvalues, the joint distribution function for the eigenvalues of positive Hermitian matrices is found for this ensemble. The asymptotic single-level density formula is derived, using a semiclassical model. It is found that the density is convex from below over most of the domain of eigenvalues. Since this is similar to the exponential dependence expected for nuclear spectra, the density is examined in a region near the level taken to correspond with the lowest nuclear level. It turns out, however, that the density is concave from below near this level, and that a large number of levels are contained in this concave region. Hence the exponential ensemble does not fairly represent nuclear energy levels, at least in this region. Various changes are made in the measure on the matrix ensemble to determine to what extent the level density depends on this measure. It is seen that the level density graph retains a characteristic shape for a wide variety of measures. The relationship of the limiting behavior of the level density for positive matrices to the semicircle law is noted.

INTRODUCTION

THERE is a hypothesis due to Wigner,[1] that one ought to be able to explain statistical relationships observed for the levels of atomic nuclei, by a mathematical treatment of distributions derived from various ensembles of matrices. This led to interesting mathematics,[2] as well as an apparently universal law of physics,[3] the nearest-neighbor spacing formula, which gives the observed repulsion of energy levels, and has been found to fit data from atomic as well as nuclear spectra. The spacing law can be derived from the Gaussian ensemble.

We will state formulas which are correct for Hermitian matrices, rather than the restricted case of real symmetric matrices. The latter are appropriate for physical systems such as nuclei, which are invariant with respect to time reversal. However, the Hermitian matrices should give results which correspond closely with the real symmetric case.[4]

For the Gaussian ensemble, the probability of finding a matrix with elements near the elements of a given n by n matrix H, is given by

$$D_n(H)\,dH = (2\pi\sigma^2)^{-(n^2/2)}2^{-(n/2)} \times \exp\left[-\mathrm{Tr}\,(H^2)/4\sigma^2\right] dH. \quad (1)$$

We let the ijth element of H be given by two real numbers, r and s.

$$h_{ij} = r_{ij} + is_{ij}, \qquad \begin{aligned} r_{ij} &= r_{ji}\,, \\ s_{ij} &= -s_{ji}. \end{aligned} \quad (2)$$

It is convenient to relabel the n^2 real parameters of H as follows. The set $\{x_1, x_2, \cdots, x_n\}$ denote the n diagonal elements r_{ii}. The set

$$\{x_{n+1}, x_{n+2}, \cdots, x_{n(n+1)/2}\}$$

denote the remaining r_{ij} with i less than j. The set $\{x_{n(n+1)/2+1}, x_{n(n+1)/2+2} \cdots x_{n^2}\}$ correspond to the $n(n-1)/2$ numbers s_{ij} with i less than j. With this notation, dH is given by

$$dH = dx_1\,dx_2 \cdots dx_{n^2}. \quad (3)$$

Rosenweig and Porter[5] proved for the real case, that if one assumes: (1) The density function is invariant under real orthogonal transformations; (2) The various matrix elements are statistically independent: then one *must* have (1) as the measure. The first requirement is a consequence of the fact that we have no reason for preferring one orthogonal basis to another. The two requirements taken together, give a nice mathematical characterization of

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[1] E. P. Wigner, Proceedings of the Gatlinburg Conference on Neutron Physics by Time of Flight, ORNL 2309, P. 67, 1956 (unpublished). See also Ref. 25.
[2] F. J. Dyson, J. Math. Phys. **3**, 140 (1962).
[3] N. Rosenzweig and C. E. Porter, Phys. Rev. **120**, 1698 (1960).
[4] M. L. Mehta and M. Gaudin, Nucl. Phys. **18**, 420 (1960). The formula derived by Mehta and Gaudin for the single level density for the real case is the same as Eq. (4) this paper, for the Hermitian case, except for normalization, and the location of the end of the semicircle. The nearest neighbor spacing for very small spacings in the real symmetric case is proportional to X, the spacing distance, while it is proportional to X^2 in the Hermitian case. See Ref. 18b and 25.
[5] C. E. Porter and N. Rosenzweig, Ann. Acad. Sci. Finnicae Ser. A VI, **44** (1960).

the ensemble, but there is no compelling reason from physics to keep the second. We will drop it in this paper.

Equation (1) leads to the semicircle law for the asymptotic single eigenvalue distribution

$$nP_n(\epsilon) = (1/8\pi\sigma^2)(8n\sigma^2 - \epsilon^2)^{\frac{1}{2}} \quad \text{for} \quad \epsilon^2 < 8n\sigma^2, \tag{4a}$$

$$nP_n(\epsilon) = 0 \quad \text{for} \quad \epsilon^2 \geq 8n\sigma^2. \tag{4b}$$

Equation (4a) has a graph which is concave from below, while one would expect for nuclear spectra that the area above the graph of the density should be convex, as it would be for an exponential function.[6] One might expect that an exact calculation in the region of transition to the tail of the distribution, [i.e., near $\epsilon = -(8n\sigma^2)^{\frac{1}{2}}$] would show this property. It was shown,[7] however, that the number of roots in this region is of the order of 2, even when the dimension of the matrices becomes very large. In this paper we will show how a level density which is convex over most of the domain of the eigenvalues can come about.

A different characterization of (1) exists. Suppose we define a density function on the space of Hermitian matrices subject to the conditions

$$\int \cdots \int D(H)\, dH = 1, \tag{5a}$$

$$\int \cdots \int x_i^2 D(H)\, dH = \begin{cases} 2\sigma^2 & i \leq n \\ \sigma^2 & i > n \end{cases}, \tag{5b}$$

$$\int \cdots \int x_i x_j D(H)\, dH = 0 \quad \text{for} \quad i \neq j. \tag{5c}$$

The limits on all integrals are $(-\infty, \infty)$ unless otherwise noted. We define an entropy function on our matrix space by

$$S \equiv -\int \cdots \int D(H) \log [D(H)]\, dH. \tag{6}$$

We will call the ensemble given by the function $D(H)$ which maximizes the entropy S subject to conditions (5), the "most random" ensemble. Shannon[8] formulated and solved this problem for slightly more general conditions than we require for our matrix ensemble. The specialization to our case gives (1).

We thus have an independent characterization of the Gaussian ensemble. We would like to see what we obtain for the "most random" ensemble when we restrict consideration to only positive, or only negative matrices, and our preliminary information consists of a common mean for all the diagonal elements. We will later compare the density of eigenvalues near the eigenvalue which is largest in magnitude, with the density of nuclear energy levels near the ground state. Therefore, at that time, we will have in mind negative Hermitian matrices. We find it easier, however, to phrase the discussion for positive matrices. Since the transformation from one case to the other simply amounts to placing a minus sign in front of the matrix and its eigenvalues, we will speak hereafter in terms of positive matrices.

The set of all complex matrices A is mapped onto the set of all positive Hermitian H by the transformation

$$A \to AA^+. \tag{7}$$

This is because any positive H can be written

$$H = UEU^+ = UE^{\frac{1}{2}}VV^+E^{\frac{1}{2}}U^+. \tag{8}$$

Here E is the diagonal matrix of the eigenvalues of H, and $E^{\frac{1}{2}}$ contains the positive square roots of these numbers. U is a unitary matrix, the columns of which are the eigenvectors of H. V is an arbitrary unitary matrix.

Let the elements of an arbitrary complex matrix A be given by $a_{ij} + ib_{ij}$ where a_{ij} and b_{ij} are real numbers. Let $D(AA^+)dA$ be the probability for finding any matrix H which can be formed by the product $(A'A'^+)$ where the real and imaginary parts of the elements of A' are in neighborhoods around the corresponding parameters for A, and

$$dA \equiv da_{11}\, da_{12} \cdots da_{nn}\, db_{11}\, db_{12} \cdots db_{nn}. \tag{9}$$

We point out that while our ensemble consists of the matrices $H = AA^+$, we are taking as our sample space the set of all complex matrices A, so that every H can be obtained in many ways. In this case we will *not* have a density function $\mathfrak{D}(H)$ calculated so that the number of matrices around H with the parameterization (2), is given as $\mathfrak{D}(H)dH$ where dH is given by (3).

We define the entropy S by

$$S \equiv -\int \cdots \int D(AA^+) \log [D(AA^+)]\, dA. \tag{10}$$

We would like to maximize S subject to

$$\int \cdots \int D(AA^+)\, dA = 1, \tag{11a}$$

$$\int \cdots \int (AA^+)_{ii}\, D(AA^+)\, dA = \mu. \tag{11b}$$

Varying D, we find the condition for stationarity

[6] T. Ericson, Phil. Mag. Suppl. 9, 425 (1960).
[7] B. Bronk, J. Math. Phys. 5, 215 (1964).
[8] C. E. Shannon, Bell System Tech. J. 27, 629 (1948).

of S

$$\delta D\{-\ln D(AA^+) - 1 + C' + \sum_i c_i(AA^+)_{ii}\} = 0, \quad (12)$$

and since δD is an arbitrary variation, we obtain

$$D(AA^+) = C^{-1} \exp\left[-\sum_i c_i(AA^+)_{ii}\right]. \quad (13)$$

C' and c_i are Lagrange multipliers corresponding to (11). Substituting D into (11a), we have the product of $2n^2$ Gaussian integrals which are evaluated to give

$$C^{-1} \prod_{i=1}^{n} \left(\frac{\pi}{c_i}\right)^{2n/2} = 1. \quad (14a)$$

Similarly, evaluation of the n integrals (11b) gives

$$\frac{2n}{2c_j} C^{-1} \prod_{i=1}^{n} \left(\frac{\pi}{c_i}\right)^{n} = \mu. \quad (14b)$$

It follows that

$$c_i = n/\mu, \quad j = 1, \cdots n; \quad C^{-1} = (n/\mu\pi)^{n^2}. \quad (15)$$

Setting μ equal to n for simplicity,

$$D(AA^+) = (\pi)^{-n^2} \exp\left[-\mathrm{Tr}\,(AA^+)\right] \quad (16)$$

is the "most random" ensemble for positive matrices when the diagonal elements have a mean equal to the dimension of the matrix. Notice that although our preliminary information as given in Eq. (11b) is not independent of the coordinate system, the form of D which we arrive at is invariant when A is subjected to a unitary transformation. This is because the Jacobian of such a transformation is one.[9] We also notice from Eq. (16) that D is everywhere less than one and therefore S is positive.

We find it interesting to consider a more general measure, still invariant under unitary transformations, which includes (16) as the simplest case.

$$D_{n,\alpha}(AA^+) = C_{n,\alpha}^{-1} \times \exp\left[-\mathrm{Tr}\,(AA^+)\right][\det\,(AA^+)]^{\alpha}, \quad (17)$$

$C_{n,\alpha}$ is a constant to be determined later. From (17) and (11a) we obtain

$$C_{n,0} = (\pi)^{n^2}, \quad (18)$$

α is a real parameter which we restrict to be greater than minus one, and much less than the dimension of H.

[9] For example, B. Bronk, thesis, Princeton University (1964). The Jacobian is explicitly calculated in Chap. 4.

2. THE n-LEVEL JOINT DISTRIBUTION FUNCTION

The method to be used in dealing with the volume element, was first worked out by Bargmann, Montgomery, and Von Neumann,[10] for real A. The complex case is given below.

An arbitrary complex matrix A can be written

$$A = U\Lambda V, \quad (19)$$

where Λ is a diagonal matrix containing the positive square roots of the eigenvalues of the Hermitian matrix AA^+, while U and V are unitary. The decomposition (19) follows from the theorem[11] that every complex matrix A can be represented

$$A = \bar{H}W, \quad (20)$$

where W is unitary, and $\bar{H}$ is a positive semidefinite Hermitian matrix which is the square root of AA^+. Hence, U is made up of column vectors which are the eigenvectors of the matrix $\bar{H} = U\Lambda U^+$, and

$$V = U^+W. \quad (21)$$

We must know to what extent U and V are determined by A. Suppose

$$U\Lambda V = U'\Lambda V' \quad (22)$$

then

$$U'^+U\Lambda = \Lambda V'V^+ \quad (23)$$

Let

$$\bar{U} \equiv U'^+U, \quad \text{and} \quad \bar{V} \equiv V'V^+, \quad (24)$$

$\bar{U}$ and $\bar{V}$ are unitary. Rewriting (23) in terms of matrix elements, we find

$$\bar{u}_{ik}\lambda_k = \lambda_i\bar{v}_{ik}. \quad (25)$$

Notice that no summation is needed in (25). Taking the absolute value squared of both sides of (25) and summing over i, we obtain

$$\lambda_k^2 = \sum_i \lambda_i^2 |v_{ik}|^2. \quad (26)$$

Now if we renumber the λ_i, and correspondingly relabel the rows of V and columns of U, we obtain

[10] (a) V. Bargmann (private communication) Bargmann, Montgomery, and Von Neumann, in their work on the early digital computers during World War II calculated with random matrices in estimating computer error. This was brought out to the author when he remarked that availability of a computer was an advantage in present work on random matrices. Bargmann's answer was "Yes, but we were designing the computers."

(b) H. H. Goldstine and J. V. Von Neumann, Am. Math. Soc. **2**, 188 (1951).

(c) S. S. Wilks, *Mathematical Statistics* (John Wiley & Sons, Inc., New York, 1962), Chap. 18 on multivariate statistics.

[11] F. R. Gantmacher, *The Theory of Matrices*, translated by K. A. Hirsh (Chelsea Publishing Company, New York, 1959), Vol. I, Chap. IX, p. 276.

the same matrix A. Therefore, we can fix attention on one ordering of the λ, and still obtain all matrices A for the given values of λ_i, as we vary U and V. To be definite we take

$$\lambda_1 > \lambda_2 > \cdots > \lambda_n. \tag{27}$$

Those cases where two eigenvalues are equal can be ignored. They are of measure zero, since they occur on a lower dimensional surface in the n-dimensional space of the eigenvalues. For the same reason, we can omit consideration of the surface $\lambda_n = 0$. Hence we only consider nonsingular A, in which case W in (20) is uniquely determined.[11] From (26) we obtain

$$\sum_i (\lambda_k^2 - \lambda_i^2) \, |\bar{v}_{ik}|^2 = 0. \tag{28}$$

Taking λ_k in (28) to be λ_1, we find since every nonzero term is then positive,

$$|\bar{v}_{i1}| = 0 \quad \text{if} \quad i \neq 1, \tag{29a}$$

$$|\bar{v}_{11}| = 1, \tag{29b}$$

but $\sum_i |\bar{v}_{1i}|^2 = 1$. Hence,

$$|\bar{v}_{1i}| = 0 \quad \text{if} \quad i \neq 1. \tag{29c}$$

Now take λ_k in (28) equal to λ_2. Then every term on the left in (28) is positive except $(\lambda_2^2 - \lambda_1^2) \, |\bar{v}_{12}|^2$ which is zero by (29). Proceeding in this manner, we find that $\bar{U}$ and $\bar{V}$ are both diagonal, with the diagonal elements having absolute value equal to one. Since U equals $U'\bar{U}$, it can only differ from U' by an arbitrary phase factor multiplying each column. Similarly, an arbitrary phase multiplies each row of V. This arbitrariness in phase, since W is unique, is wholly contained in U. It reflects the fact that the left-hand side of Eq. (19) is described by $2n^2$ parameters, while for the right-hand side we need $2n^2 + n$ parameters. Weyl[12a] considered this problem in connection with defining the volume element for the unitary group. The solution is to form an equivalence class of all unitary matrices belonging to the right coset of an element of T, where T is the set of all diagonal matrices of the form

$$||e^{i\tau_k}|| \qquad k = 1, \cdots n. \tag{30}$$

The $(n^2 - n)$-dimensional manifold thus formed is denoted $[U(n)]$ and its elements are given by $[U]$. In our case we consider the transformation

$$A \to [U] \, \Lambda \, V, \tag{31}$$

V varies over all elements of the n-dimensional unitary group Un. If $V + dV$ is a unitary matrix varying over a neighborhood about V, then a volume element for this neighborhood which is invariant over the unitary group is given by the product[13]

$$\prod_{i<k} dt_{ik} \prod_{i \leq k} dv_{ik}, \tag{32}$$

where dt_{ik} and dv_{ik} are the real and imaginary parts of the ikth element of the skew Hermitian matrix

$$\delta V \equiv V^{-1} \, dV \tag{33}$$

Correspondingly, to define a neighborhood around $[U]$, we remember that $U + dU$ is equivalent to $(U + dU)(\mathbb{1} + id\tau)$, where $id\tau$ gives n infinitesimals corresponding to the exponents for an element of T, which happens to be close to $\mathbb{1}$. Now

$$\delta U = U^{-1} \, dU \tag{34}$$

and by the above we have the equivalency

$$\delta U = \delta' U = (\delta U + i \, d\tau). \tag{35}$$

Since the diagonal elements of the skew Hermitian δU are pure imaginary, we may choose $d\tau$ so as to make them exactly zero, but the off-diagonal elements are unaffected by $d\tau$. If the ikth element of δU is given by $dr_{ik} + ids_{ik}$, we take for the volume element of $[U(n)]$ at $[U]$,

$$\prod_{i<k} dr_{ik} \prod_{i<k} ds_{ik}. \tag{36}$$

For T_0 an element of T, we must have, by our equivalence relation, the volume for UT_0 the same as for U, since when we move from U to $U + dU$, in $[U(n)]$, this is the same as moving from UT_0 to $(U + dU)T_0$. This has been established by Weyl.[12a] It is also found[14] that the volume element (36) is invariant in $[U(n)]$, and it is shown[14] that

$$\Omega_{[U]} = \Omega_U/(2\pi)^n, \tag{37}$$

where $\Omega_{[U]}$ is the total volume for $[U(n)]$ and Ω_U is the volume for the n-dimensional unitary group.

A straightforward calculation[15] shows that if U_0 is a fixed unitary matrix, the transformation

$$A \to U_0 A \tag{38}$$

has a Jacobian equal to one, and therefore the Jacobian of the transformation (31), may be calculated for U and V both close to the unit element.

Hence to evaluate the Jacobian, J, of (31), we

[12] (a) H. Weyl, *The Classical Groups* (Princeton University Press, Princeton, New Jersey, 1939) p. 194.
(b) L. K. Hua, *Harmonic Analysis of Functions of Several Complex Variables* (Am. Math. Soc., Providence, Rhode Island, 1963), Chap. III, An alternate derivation, also based on Ref. 12a, of a formula corresponding to (42) is given here.

[13] D. E. Littlewood, *The Theory of Group Characters* (Oxford University Press, Oxford, England, 1940), Chap. XI.

[14] Cf. Ref. 12a; also Ref. 9, Appendix 4.

[15] Cf. Ref. 9, Chap. 4.

look at

$$A + dA = (\mathbb{1} + dU)(\Lambda + d\Lambda)(\mathbb{1} + dV). \tag{39}$$

As explained above, the diagonal elements of dU are taken equal to zero. Equating real and imaginary parts of the differential elements in (39), we obtain

$$\begin{aligned} da_{ii} &= d\lambda_{ii}, & db_{ii} &= \lambda_i\, dv_{ii}, \\ da_{ij} &= dr_{ij}\lambda_j + \lambda_i\, dt_{ij}, & db_{ij} &= ds_{ij}\lambda_j + \lambda_i\, dv_{ij}, \\ da_{ji} &= -dr_{ij}\lambda_i - \lambda_j\, dt_{ij}, & db_{ji} &= ds_{ij}\lambda_i + \lambda_j\, dv_{ij}. \end{aligned} \tag{40}$$

J is the absolute value of the $2n^2$ by $2n^2$ determinant obtained from the coefficients of the right-hand side of (40). It breaks down into the product of an n-dimensional unit determinant, the n-dimensional determinant of Λ, and $2n(n-1)$ two-dimensional determinants of the form

$$\pm \begin{vmatrix} \lambda_j & \lambda_i \\ \lambda_i & \lambda_j \end{vmatrix} = \pm(\lambda_j^2 - \lambda_i^2), \tag{41}$$

giving[12b]

$$J(\Lambda) = \prod_{i<j} (\lambda_i^2 - \lambda_j^2)^2 \prod_i \lambda_i. \tag{42}$$

Integrating expression (17) over Un and $[U(n)]$, and transforming to $\epsilon_i = \lambda_i^2$, we obtain with (31) and (42),

$$P_{n,\alpha}(\epsilon_1, \epsilon_2, \cdots, \epsilon_n)\, d\epsilon_1 \cdots d\epsilon_n = (2^n n!)^{-1} \Omega_U \Omega_{[U]}$$

$$\times \exp\left[-\sum \epsilon_i\right] \prod_{i=1}^{n} \epsilon_i^{\alpha} \prod_{i<j} (\epsilon_i - \epsilon_j)^2\, d\epsilon_1 \cdots d\epsilon_n, \tag{43}$$

$P_n(\epsilon_1, \epsilon_2, \cdots, \epsilon_n)$ is the n-level joint distribution function. The $n!$ in the denominator of the right-hand side is due to the fact that we now allow all orderings of the $\{\epsilon_i\}$, whereas up to now we ordered the eigenvalues. The factor 2^n, is from the last change of variables.

The factor $\prod_{i<j} (\epsilon_i - \epsilon_j)^2$ is the square of the Vandermonde determinant Δ, where

$$\Delta = \begin{vmatrix} 1 & 1 & \cdots & 1 \\ \epsilon_1 & \epsilon_2 & \cdots & \epsilon_n \\ \vdots & & & \\ \epsilon_1^{n-1} & \epsilon_2^{n-1} & \cdots & \epsilon_n^{n-1} \end{vmatrix}. \tag{44}$$

We will make use of the associated Laguerre polynomials, which are orthogonal with respect to the weight $(e^{-x}x^{\alpha})$, on the positive half line. α is real, and greater than minus one. The Rodrigues formula[16] for these polynomials is

$$L_n^{\alpha}(x) \equiv \frac{1}{n!} e^x x^{-\alpha} \frac{d^n}{dx^n} (e^{-x} x^{n+\alpha}), \tag{45}$$

where n is the order of the polynomial. The normalization is given by

$$\int_0^{\infty} e^{-x} x^{\alpha} [L_n^{\alpha}(x)]^2\, dx = \Gamma(\alpha + 1) \binom{n+\alpha}{n}. \tag{46}$$

The second factor on the right is a binomial coefficient.

Since we can add linear combinations of the other rows to a given row in (44) without changing the value of Δ, with (45) we obtain

$$\Delta = \left[\prod_{m=0}^{n-1} (m!)\right] \begin{vmatrix} 1 & 1 & \cdots & 1 \\ L_1^{\alpha}(\epsilon_1) & L_1^{\alpha}(\epsilon_2) & \cdots & L_1^{\alpha}(\epsilon_n) \\ \vdots & & & \\ L_{n-1}^{\alpha}(\epsilon_1) & L_{n-1}^{\alpha}(\epsilon_2) & \cdots & L_{n-1}^{\alpha}(\epsilon_n) \end{vmatrix}. \tag{47}$$

If

$$\phi_k(\epsilon) = e^{-\epsilon/2} \epsilon^{\alpha/2} L_k^{\alpha}(\epsilon) \left[\Gamma(\alpha + 1) \binom{n+\alpha}{n}\right]^{-\frac{1}{2}}, \tag{48}$$

then

$$P_n(\epsilon_1, \cdots \epsilon_n) = K \begin{vmatrix} \phi_0(\epsilon_1) & \phi_0(\epsilon_2) & \cdots & \phi_0(\epsilon_n) \\ \vdots & & & \\ \phi_{n-1}(\epsilon_1) & \phi_{n-1}(\epsilon_2) & \cdots & \phi_{n-1}(\epsilon_n) \end{vmatrix}^2, \tag{49}$$

$$K = C_{n,\alpha}^{-1} \Omega_{U_n} \Omega_{[U(n)]} [\Gamma(\alpha + 1)]^n$$

$$\times \left[\prod_{m=1}^{n-1} \binom{m+\alpha}{m}\right] \left[\prod_{m=0}^{n-1} (m!)\right]^2 (2^n n!)^{-1}. \tag{50}$$

Now if we call the determinantal factor in (49), Δ'^2, then we can see directly that the n-level joint distribution function normalized to one is

$$P_n(\epsilon_1, \cdots, \epsilon_n) = (n!)^{-1} \Delta'^2. \tag{51}$$

That this normalization is correct is evident from the single level density formula

$$P_n(\epsilon) = (1/n) \sum_{k=0}^{n-1} \phi_k^2(\epsilon). \tag{52}$$

This familiar result is obtained by expanding the first Δ' in (51) along the first column, and integrating $P_n(\epsilon_n, \cdots, \epsilon_1)$ over all but the first ϵ. The range of integration is $(0, \infty)$. The minor corresponding to ϕ_i expands into $(n-1)!$ terms, each of which is orthogonal to all but the corresponding term from ϕ_i's minor from the second Δ', and integrates with that term to give one.

[16] Bateman Manuscript Project, edited by A. Erdélyi, (McGraw-Hill Book Company, Inc., New York, 1953). Sec. (10.12), Eqs. (5) and (2).

We can now evaluate the normalization constant, $C_{n,\alpha}$. Setting α in (50) equal to zero, and using (18) and (51) we have

$$\Omega_{U_n}\Omega_{[U(n)]} = \left\{\frac{2^n\Pi^{n(n+1)/2}}{\prod_{m=0}^{n-1} m!}\right\}\left[\frac{2^n\Pi^{n(n+1)/2}}{(2\pi)^n\prod_{m=0}^{n-1} m!}\right]. \quad (53)$$

The value for Ω_{U_n} given by the first term on the right may be checked against the value obtained by Dyson[17] in another way. Using (53) with (50) and (51), we have $Kn! = 1$, hence

$$C_{n,\alpha} = \Pi^{n^2}[\Gamma(\alpha+1)]^n\left[\prod_{m=1}^{n-1}\binom{m+\alpha}{m}\right]. \quad (54)$$

3. SEMICLASSICAL DERIVATION OF THE ASYMPTOTIC SINGLE LEVEL DENSITY

We will use the phase space of the hydrogen atom to find the asymptotic single level density. This corresponds to the use of the harmonic oscillator[18] in the investigation of the Gaussian ensemble.

Consider the radial equation[19] for a hydrogen atom with angular momentum $\ell\hbar$.

$$(-\hbar^2/2\mu)[1/r^2\,(d/dr)(r^2\,d/dr) - \ell(\ell+1)/r^2]R_{m\ell}(r) - (e^2/r)R_{m\ell}(r) = E_m R_{m\ell}(r). \quad (55)$$

If

$$r = (m\hbar^2/2\mu e^2)\rho \quad \text{and} \quad (-2E) = (\mu e^4/m^2\hbar^2) \quad (56)$$

then we obtain

$$\left[1/\rho^2\,(d/d\rho)(\rho^2\,d/d\rho) - \frac{1}{4} + \frac{m}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]R_{m\ell}(\rho) = 0. \quad (57)$$

The classical equation of motion corresponding to (55) is

$$p_r^2/2\mu + p_\phi^2/2\mu r^2 - e^2/r = E. \quad (58)$$

If

$$p_\rho^2 = [-1/4 + m/\rho - \ell(\ell+1)/\rho^2] \quad (59)$$

then using (56),

$$p_\rho = (-1/2E)^{\frac{1}{2}}(1/4\mu)^{\frac{1}{2}}p_r. \quad (60)$$

The quantum condition

$$\oint p_r\,dr = (m-\ell)h \quad (61)$$

gives us using (56) and (60),

$$\oint p_\rho\,d\rho = 2\pi(m-\ell). \quad (62)$$

The functions satisfying (57) and the orthonormalization

$$\int_0^\infty R_{m\ell}R_{m'\ell}\rho^2\,d\rho = \delta_{m'm} \quad (63)$$

are

$$R_{n\ell}(\rho) = \text{const}\;\rho^\ell e^{-\rho/2}\mathfrak{L}_{m+\ell}^{2\ell+1}(\rho). \quad (64)$$

The $\mathfrak{L}_{m+\ell}^{2\ell+1}(\rho)$ are the polynomials of order $(m-\ell-1)$ defined by (63) and (64). The Rodrigues formula[20] for these polynomials is

$$\mathfrak{L}_n^m(\rho) = (-)^m(n!/(n-m)!) \times e^\rho\rho^{-m}d^{n-m}/d\rho^{n-m}(e^{-\rho}\rho^n). \quad (65)$$

If we look at the derivation of (52), we see that we can write for the single level density,

$$P_{n,\alpha}(\rho)\,d\rho = \left\{1/n\sum_{m=\ell+1}^{n+\ell}[R_{m\ell}\rho]^2\right\}d\rho \quad (66)$$

where we have taken

$$\alpha = 2(\ell+1); \qquad \epsilon = \rho. \quad (67)$$

The form we obtain for the level density will apply to more general α than the even integers we consider explicitly. Since the wavefunctions are more closely confined to their classical orbits when m is large,[21] we will obtain a better asymptotic approximation to the level density if we restrict ourselves to $1 \ll \ell$. This is particularly true for the smaller allowed values of ρ, where the orbits are crowded close together.

The right-hand side of (66) gives the probability that a particle, which is with equal weight in the first n quantum states of angular momentum ℓ, will be found between ρ and $\rho + d\rho$. The first few even orbits of the corresponding classical phase space are shown in Fig. 1. The top half of the graph for a given value of m is indicative of the form of the eigenvalue density which we obtain below.

Now since we are considering Eq. (66) for cases where the quantum numbers m are large, we can consider it as giving the probability density for a

[17] Reference 2, Eqs. (106) and (108).

[18] (a) E. P. Wigner, "Distribution Laws for Roots of a Random Hermitian Matrix" (unpublished). Some results of this work are available in:
(b) N. Rosenzweig, *Brandeis Summer Institute 1962, Statistical Physics* (W. A. Benjamin, Inc., New York, 1963); Mehta and Gaudin's derivation of the spacing formula for the real case is also shown here.

[19] Cf., L. P. Landau and L. M. Lifshitz, *Quantum Mechanics Non-Relativistic Theory*, translated by Sykes and Bell, (Pergamon Press, Ltd., London, 1958), Paragraph 36.

[20] Reference 19, Appendix d.

[21] Reference 19, Chap. VII, see footnote p. 157.

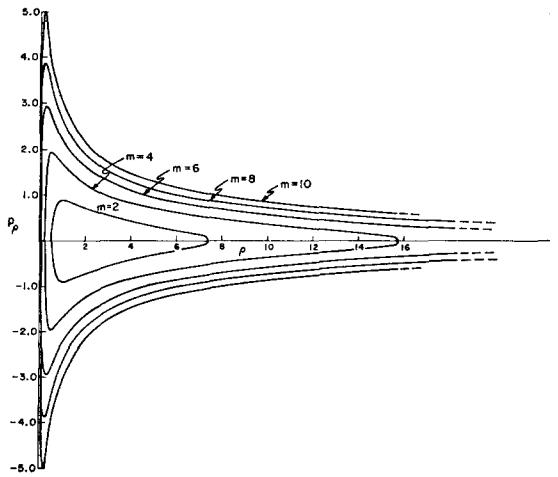

FIG. 1. The first few even orbits in phase space of hydrogen atom for $\ell = \ell$.

classical particle which is with equal probability on each of the first n orbits of angular momentum ℓ, in the phase space of ρ and p_ρ. According to Liouville's theorem of classical statistical mechanics, equal areas of our two-dimensional phase space have equal probability, and the probability density is proportional to $(dp_\rho d\rho)$. If we integrate over p_ρ, we obtain the density in ρ,

$$P_{n,\ell}(\rho) = \left(\frac{1}{\pi n}\right)\left(\frac{n+\ell}{\rho} - \frac{\ell^2}{\rho^2} - \frac{1}{4}\right)^{\frac{1}{2}}$$

$$\text{for} \quad \frac{\ell^2}{(n+\ell)} \leq \rho \leq 4n + 4\ell, \qquad (68)$$

$$P_{n,\ell}(\rho) = 0 \quad \text{otherwise.}$$

The normalization constant is obtained from Eq. (62) or from actual evaluation of the integral of (68) over ρ, as in Ref. 22.

4. DISCUSSION

Let us discuss the general features of the level density as given by (68). $P_n(\rho)$ has only one maximum which is located at $\rho = [2\ell^2/(n+\ell)]$. The derivative of the level density becomes infinite at $\rho_{\max} = 4n + 4\ell$, and $\rho_{\min} = [\ell^2/(n+\ell)]$.

If α is greater than one, it is easy to see from (48) and (52), that both $P_n(\rho)$ and its first derivative are zero at the origin, so that a convex region[23] exists between the origin and $\rho_{\min}$. If ℓ is a fixed constant, and n is increasing, the maximum at $(2\ell^2/n)$ may for all practical purposes be considered to be at the origin. In this case, we can write an approximation for (68) valid over most of its range, in which the ℓ dependence has been removed.

$$P_n(\rho) \approx (1/\pi n\rho^{\frac{1}{2}})(4n - \rho)^{\frac{1}{2}} \quad \text{for} \quad 0 < \rho \leq 4n \qquad (69)$$
$$P_n(\rho) = 0 \quad \text{otherwise.}$$

In this case, we might as well set α equal to zero in order to investigate the general properties of the density. Doing this, we find the exact value of the density at ℓ equals zero from (48) and (52).

$$P_{n,0}(0) = 1. \qquad (70)$$

Since, from (45), the coefficient of the lowest power of x in $L_n(x)$ is of opposite sign from the constant term, the slope of P_n is negative at the origin. The asymptotic expression for P_n has two points of inflection away from the origin, one is found at the zero of the second derivative of (69), and is at

$$\rho = 3n. \qquad (71)$$

If we used (68) for $\ell \neq 0$, we would find this inflection point at $\rho = 3(n+\ell)$. At this point, the graph of the density which was convex nearer the origin, becomes concave, until a second point of inflection is reached near ρ equals $4n$. We know the existence of this point from the fact that the exact expression for P_n is never zero. We will temporarily return to the use of the more accurate expression (68), to see what happens to the two additional inflection points on each side of the maximum of P_n. The numerator of the second derivative of (68) is

$$N = -4n'\rho^3 + 12(\ell^2 + n'^2)\rho^2 - (48\ell^2 n' - 4\ell^2)\rho + 32\ell^4, \qquad (72)$$
$$n' \equiv (n+\ell).$$

If we assume $(\ell^4/n) \to 0$, and set N equal to zero, we get a cubic equation, which can be factored to obtain

$$\rho = 0,$$
$$\rho = (4\ell^2/n'), \qquad (73)$$
$$\rho = 3n'.$$

The third point corresponds to the one we already obtained from (69). The first we knew should be at zero, since the maximum approaches zero, and we can see that the remaining inflection point at $(4\ell^2/n')$ also approaches arbitrarily close to zero, as n' becomes very large.

[22] M. Born, *Mechanics of the Atom*, translated by Fisher & Hartree (G. Bell and Sons, London, 1960), Appendix II.

[23] It is shown in this paper that the convex region near the origin is unimportant for fixed ℓ. However, the "strong" case in which $\ell \to \infty$ as a certain power of n, may be different and will be investigated in a later paper.

[24] See Ref. 9, Chap. 5.

The number of roots which occur in the region beyond ρ equals $4n$ can be estimated by comparison with the corresponding calculation for the Gaussian ensemble. This is done explicitly in Ref. 9 and it is found that the number of roots in this region is negligible, when α is much smaller than n, even when n becomes very large.

Now we can see that the region containing the largest number of levels is where the argument ρ (always positive) of the single level density formula is small. We might therefore expect ρ to represent minus the energy, as it would for negative matrices. If this were the case, the region corresponding to the lowest energies would be where ρ is large. In this region, we have found that the level density is slightly concave, increasing slowly from that near the first level until the inflection point is reached beyond which the growth becomes increasingly rapid as the curve enters the convex region. Although most of the roots occur in the convex region, as one would expect for nuclear energy levels, it is easy to see from Eq. (69), that the number of roots in the concave region, that is

$$\int_{3n}^{4n} nP_n(\rho)\, d\rho, \tag{74}$$

grows as the first power of n. This region corresponds to the concave portion (near $x = 4$), of the curve labeled $n = 6$ (asymptotic), in Fig. 2, although this drawing is for a somewhat different measure. Hence, the density of the roots which we have taken as corresponding to the low-lying energy levels, does not show a convex growth as expected for nuclear level densities. Therefore, the ensembles discussed here, do not fairly represent nuclear Hamiltonians, at least in this region.

We should mention that the repulsion of levels follows from the term $\prod_{i<j} (\epsilon_i - \epsilon_j)^2$ in (43). It is easy to show that the dependence of the nearest-neighbor spacing density function on the distance between nearest neighbors, is the same as for the Gaussian ensemble, at least to first order, in a region where the level density varies slowly. Leff[25a] previously pointed out that this also holds when Legendre functions are the normalized functions[25c] in Eq. (52).

[25] (a) H. Leff, thesis, State University of Iowa, (SUI 63-23), p. 105 (1963) (unpublished), see also (b) D. Fox and P. B. Kahn, Phys. Rev. 134, B 1151 (1964). (c) P. Kahn, C. E. Porter, and Y. C. Tang (to be published). This group has been investigating various aspects of functions obtained by inserting different sets of orthogonal functions into Eq. (52). Their numerical result for the Laguerre functions confirms the convex shape obtained here.

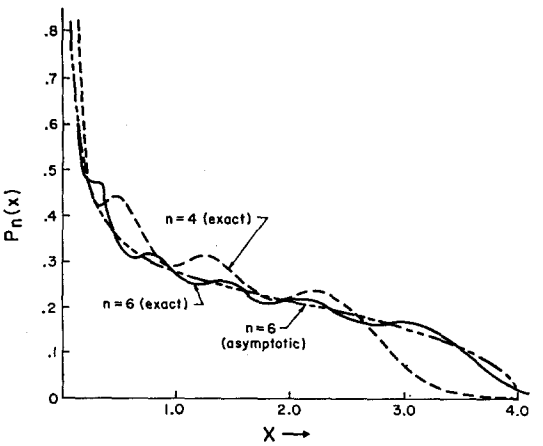

FIG. 2. Single eigenvalue density for Gaussian ensemble, over positive matrices. Graph labeled asymptotic is for Eq. (84). The other graphs are Eq. (52) with the functions ϕ_k coming from the orthonormalization of set (80).

Relation of the Level Density to the Semicircle Law

In Eq. (69), suppose we let $\rho^{\frac{1}{2}} = y$. Then we obtain for the density of the square roots of the eigenvalues

$$\tilde{P}_n(y)\, dy = (2/n\pi)(4n - y^2)^{\frac{1}{2}}\, dy \quad \text{for} \quad 0 \leq y \leq 4n,$$
$$= 0 \quad \text{otherwise.} \tag{75}$$

So we are brought back to the positive half of a semicircle for the positive square roots of the eigenvalues.

We can obtain (75) directly in the space of the square roots of the eigenvalues, if we analyze the special case of $\alpha = -\frac{1}{2}$. In this case, from (42) and (43) we obtain,

$$P_{n,-\frac{1}{2}}(\lambda_1, \lambda_2, \cdots, \lambda_n)\, d\lambda_1 \cdots d\lambda_n$$
$$= \text{const.} \exp\left[-\sum_{i=1}^{n} \lambda_i^2\right]$$
$$\times \prod_{i<j} (\lambda_i^2 - \lambda_j^2)^2\, d\lambda_1 \cdots d\lambda_n, \tag{76}$$

where λ_i are the positive square roots of an n-dimensional random positive matrix distributed according to (17) with α equal to $(-\frac{1}{2})$. The product term in (76) can be written

$$\Delta^2 = C \begin{vmatrix} H_0(\lambda_1) & H_0(\lambda_2) & \cdots & H_0(\lambda_n) \\ H_2(\lambda_1) & H_2(\lambda_2) & \cdots & H_2(\lambda_n) \\ \vdots & & & \\ H_{2n-1}(\lambda_1) & H_{2n-2}(\lambda_2) & \cdots & H_{2n-2}(\lambda_n) \end{vmatrix}^2. \tag{77}$$

The entries in the determinant in (77) are the even Hermite polynomials. Since the *even* polynomials are orthogonal with respect to $(e^{-\lambda_i^2})$ on the *half* line,

we obtain as previously, by integrating over all but one column of Δ,

$$P_{n,-\frac{1}{2}}(\lambda) = (2/n) \sum_{\substack{i=0 \\ \text{even}}}^{2n-2} \phi_i^2(\lambda), \tag{78}$$

where $\phi_i(\lambda)$ is the Hermite function normalized on the whole line. Now we can use Wigner's[18] analysis of the phase space of the harmonic oscillator, and we again arrive at (75).

Invariance Properties

It is of interest to ask, to what extent the properties of our ensemble depend on the fact that we have restricted our domain to positive Hermitian matrices, and to what extent the level density depends on the precise invariant measure chosen for our ensemble. We will first see what happens when we rewrite (17) with a Gaussian-like measure, but still over positive matrices.

$$D(AA^+)\, dA \equiv C' \exp\left[-\mathrm{Tr}\,(AA^+)^2\right] dA. \tag{79}$$

In this case, Eq. (52) still gives the single eigenvalue density, except that ϕ_i now represents the ith function obtained when a Gram–Schmidt orthonormalization on the *half* line is carried out on the set

$$\{e^{-\epsilon^2/2},\ \epsilon e^{-\epsilon^2/2},\ \cdots,\ \epsilon^{n-1}e^{-\epsilon^2/2}\}. \tag{80}$$

These functions do not relate to a known differential equation, and are difficult to tabulate even numerically owing to polynomials in $\pi^{\frac{1}{2}}$ in the coefficients. Numerical plots of the density for the matrix dimension, n equals 4, and 6, are shown in Fig. 2. A curve of the asymptotic formula derived below is plotted on the same graph for n equals 6. The closeness of the fit to the exact density shows that the asymptotic methods used become valid for rather small n.

If we start with (79) as our measure, we obtain for the joint distribution function

$$P(\epsilon_1, \epsilon_2, \cdots, \epsilon_n) = \text{const} \prod_{i<j} (\epsilon_i - \epsilon_j)^2 \sum_i e^{-\epsilon_i^2}. \tag{81}$$

Except for the fact that the ϵ_i in the present case are restricted to the positive half-line, this is the same expression studied by Wigner[26] in connection with the Gaussian ensemble. It is argued that the right-hand side of (81) is the classical distribution function for a set of n point charges interacting among themselves with a logarithmic repulsive potential, and attracted to the origin with a harmonic oscillator potential. We define a density $\sigma(\lambda)$ for these charges. Then it is assumed as in classical statistical mechanics, that the charges distribute themselves in such a way as to maximize the logarithm of the joint distribution function. This is equivalent to the usual statement that the overwhelming majority of states for a classical system are very near to the most probable state. The variational calculation of Ref. 26 leads to the integral equation correct for the present case

$$\int_0^A \frac{\sigma(\mu)}{(\lambda - \mu)}\, d\mu = \lambda. \tag{82}$$

The integral in (82) is by definition a principal-value integral. The equation is valid for $0 \leq \lambda \leq A$. This equation and the fact that the density σ, is never negative, determine σ. A is determined from the condition

$$\int_0^A \sigma(\mu)\, d\mu = n. \tag{83}$$

The solution of (82) is given by

$$\begin{aligned} nP_n(\mu) &= \sigma(\mu) \\ &= (1/\pi)(\tfrac{1}{2}A + \mu)(A - \mu)^{\frac{1}{2}}\mu^{-\frac{1}{2}} \quad \text{for} \quad \mu < A, \\ nP_n(\mu) &= 0 \quad \text{otherwise.} \end{aligned} \tag{84}$$

To verify that (84) is the correct solution,[27] we use the well-known identity

$$\lim_{\epsilon \to 0} \int_0^A \frac{d\mu\sigma(\mu)}{(\mu - (\lambda + i\epsilon))} = \pi i\sigma(\mu) + \int_0^A \frac{d\mu\sigma(\mu)}{(\mu - \lambda)}. \tag{85}$$

The integral on the right is again a principal value.

Now using (84) for σ, we evaluate the left-hand side of (85) by integrating clockwise along a contour C surrounding the cut between zero and A, but coming between the pole at $(\lambda + i\epsilon)$ and the cut.

$$\int_0^A \frac{d\mu\sigma(\mu)}{(\mu - (\lambda + i\epsilon))} = -\frac{1}{2}\int_C \frac{d\mu\sigma(\mu)}{(\mu - (\lambda + i\epsilon))}. \tag{86}$$

The factor $\frac{1}{2}$ comes from the fact that the phase of the integrand changes by exactly π, from below the cut, to above. To evaluate (86) it is convenient to use the transformations

$$\mu = A(1 + x)/2, \quad \text{then,} \quad x = 1/z. \tag{87}$$

We then notice that the only contributions come from poles at $(\lambda + i\epsilon)$, and at z equals zero, which are inside the contour after inversion. The residue

[26] E. P. Wigner, *Statistical Properties of Real Symmetric Matrices with Many Dimensions*, Proceedings of the Canadian Mathematical Congress (1957), p. 174.

[27] Actually (84) was first found by using a general solution for singular equations like (82) found in, S. G. Mikhlin, *Integral Equations* (Pergamon Press, Inc., New York, 1957), p. 131. Thanks are due to H. Leff for this reference and J. Noble for instructive discussion on such integral equations.

at $(\lambda + i\epsilon)$ gives the first term of (85), while from the residue at z equals zero, we get λ, which is the right-hand side of (82). If we substitute (84) into (83), we obtain

$$A = (8n/3)^{\frac{1}{2}}. \tag{88}$$

Now $P_n(\mu)$ as given by (84), appears somewhat different from (69), however the graphs of the two expressions have similar shapes. The graph obtained from (84) is convex from the origin until an inflection point is reached at μ equal to $A/2$. Then it is concave until μ equals A, where the exact expression for P_n must have a second inflection point. We note that if A' equals $4n$, the first inflection point for (69) occurs at $(3A'/4)$, and the second at A'.

Another type of change of measure may be considered by starting with (17), but letting ℓ as defined in (67) vary with n. Let

$$\ell = cn^{\gamma}, \tag{89}$$

γ is a positive real number which we restrict to be less than one, so $\ell/n \to 0$ as $n \to \infty$. We take the constant c equal to one. Let us discuss what happens to expression (68), in three cases, which we name to correspond with the size of the charge at the origin, when we use the electrostatic interpretation of the joint distribution function described earlier. The cases are:

(1) Weak $\gamma < \frac{1}{2}$;

(2) Critical $\gamma = \frac{1}{2}$;

(3) Strong $\frac{1}{2} < \gamma < 1$.

The situation in the weak case is very much the same as in the case for fixed ℓ, with the maximum of the distribution approaching the origin as n becomes very large. When γ equals $\frac{1}{2}$, the situation changes, and the maximum is located at ρ equal to 2. For the strong charge, we note that the entire nonzero portion of (68) is pushed increasingly far to the right, as γ increases. We obtain a family of density functions for the different γ, each peaked at $2n^{2\gamma-1}$. If we were to take a linear combination of ensembles with different coefficients for various γ, we see that we can approximate closely, an arbitrary single level density formula. If each of these ensembles has the same dimension n, we still have repulsion of the levels. We will not pursue these linear combinations further, since we do not have at present any physical motivation for assigning weights to the γ's. The exact level density between ρ equals zero and $\ell^2/(n + \ell)$ needs to be more closely examined[23] since it may be that the convex region located here in the strong case will contain sufficient roots to be used as a model for nuclear level densities.

We have found, by examining several examples, that the eigenvalue density for positive matrices while not invariant with respect to the measure chosen, retains certain general features for a variety of possible measures.

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Reduced Density Matrices of Quantum Gases. I. Limit of Infinite Volume

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The reduced density matrices for quantum gases are studied by Banach space techniques. For suitably restricted interactions, they are shown to be analytic functions of the activity. As the volume of the system becomes infinite, they tend in some sense to well-defined limits for which the same analyticity properties hold. As a consequence, the virial expansion is shown to be convergent in a neighborhood of the origin.

INTRODUCTION

RECENTLY the correlation functions of classical gases and the convergence of the virial expansion have been studied, in the limit of infinite volume, by Banach space techniques (Ref. 1, see also Refs. 2, 3). The purpose of the present paper is to study the analogous problem in quantum mechanics, by similar methods. More precisely, we prove that the reduced density matrices, which are the quantum analogues of the correlation functions, tend in some sense to well-defined limits when the volume of the system becomes infinite. We use the formalism of the grand canonical ensemble and restrict ourselves to systems of particles interacting by two-body forces only. The two-body potential will be supposed to satisfy certain conditions, stated in Sec. 1. We shall consider successively (a) the quantum mechanical problem with Maxwell–Boltzmann (MB) statistics; (b) The quantum mechanical problem with quantum statistics. The reason for doing so is that the former case is much simpler, constitutes an intermediate step, and allows us to split the difficulties. Furthermore, we reach similar conclusions in both cases under conditions on the potential which are weaker in the MB case than in the full quantum case.

The basic tool of the present investigation is Wiener integration. The relevant definitions and properties will be found in Appendix 1, which follows closely Ref. 4 and stresses only the minor modifications needed for the present application.

Sections 2 to 4 deal with the case of Maxwell–Boltzmann statistics. The reduced density matrices are introduced in Sec. 2 and shown to be expressible as Wiener integrals over suitable functionals. These functionals are shown to satisfy a set of linear integral equations, similar to the classical Kirkwood Salzburg equations,[5] and which can be viewed as a linear equation in a Banach space (Sec. 3). It is then possible to perform the limit of infinite volume, first on the intermediate functionals, and then on the density matrices themselves (Sec. 4).

Sections 5 to 7 deal with the full quantum-mechanical case and treat the same points in the same order.

1. CONDITIONS ON THE POTENTIAL

We consider a system of identical particles in ν-dimensional Euclidian space, interacting through a two-body potential Φ with the following properties:

(a) Φ is a real function which depends only on the difference of the positions of the two interacting particles considered, and is a symmetric function of these two particles.

In view of the use of Wiener integration, we impose

(b) There is a closed set F of capacity 0 (see Appendix 1) such that Φ is continuous on the complement of F.

This implies (Appendix 1) that the Wiener measure of the trajectories which intersect F is zero. Therefore we will be able to proceed as if Φ were continuous. On the other hand, this allows for instance, for $\nu > 1$, a singularity at the origin, which may have physical interest.

(c) Φ is integrable in the whole space.

$$\int |\Phi(x)|\, dx < +\infty . \tag{1.1}$$

Note that (b) and (c) exclude hard-core potentials.

(d) In the case of Maxwell–Boltzmann statistics: There exists a real constant $B \geq 0$ such that for

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[1] D. Ruelle, Ann. Phys. (N. Y.) **25**, 109 (1963).

[2] O. Penrose, J. Math. Phys. **4**, 1312 (1963).

[3] J. L. Lebowitz and O. Penrose, J. Math. Phys. **5**, 841 (1964).

[4] E. Nelson, J. Math. Phys. **5**, 332 (1964).

[5] T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956).

any system of different points $x_i \in R^\nu$ $(i=1, \cdots, n)$,

$$\sum_{i<j} \Phi(x_i - x_j) \geq -nB. \tag{1.2}$$

This implies in particular that Φ is bounded from below by $-2B$. Ruelle[6] has given sufficient conditions for (1.2) to hold.

(d′) In the case of quantum statistics only: $\Phi(x) \geq 0$. This means that the potential is purely repulsive, and is a severe physical limitation.

2. THE REDUCED DENSITY MATRICES FOR MAXWELL-BOLTZMANN STATISTICS

The system is supposed to be enclosed in a bounded (open) region Λ with volume V. We use units such that $\hbar = 1$ and that the common mass of the particles be 2. We note $\beta = 1/kT$, $\lambda = (\pi\beta)^{\frac{1}{2}}$, thermal wavelength, and z = activity. Points in R^ν are denoted by x, y, u, v and trajectories by ω. $\bar{\omega}$ means always that the corresponding trajectory is an integration variable. Upper indices in x^m (or ω^m) denote systems of m ν-dimensional points (or trajectories) while lower indices label individual members of such systems. We define

S^m = the set of families of m continuous trajectories in R^ν, $(S^1 = S)$;

S^m_Λ = the subset of S^m consisting of the trajectories contained in Λ^m, $(S^1_\Lambda = S_\Lambda)$;

$\alpha_\Lambda(\omega^m)$ = characteristic function of S^m_Λ.

$$\psi_\beta(x^m - y^m) = \prod_{i=1}^{m} \frac{1}{\lambda^\nu} \exp\left[-\frac{1}{\beta}(x_i - y_i)^2\right];$$

$$U_m(\omega^m) = \int_0^\beta \sum_{1\leq i<k\leq m} \Phi[\omega_i(t) - \omega_k(t)]\, dt. \tag{2.1}$$

It follows from (1.2) that

$$U_m(\omega^m) \geq -m\beta B. \tag{2.2}$$

The Wiener integral (Appendix 1) of a functional $f(\omega^m)$ is denoted $\int P_{x^m,y^m}(d\omega^m) f(\omega^m)$. Let $H_m(x^m, y^m)$ be the m-particle Hamiltonian operator corresponding to the box Λ. It is shown in Appendix 1 that

$$e^{-\beta H_m}(x^m, y^m) = \int P_{x^m,y^m}(d\omega^m)\alpha_\Lambda(\omega^m) \times \exp[-U_m(\omega^m)] \tag{2.3}$$

and that this quantity is a continuous function of x^m, y^m (except when one of the $x_i - x_k$ or $y_i - y_k$ lies in F), bounded by

$$e^{\beta m B}\psi_\beta(x^m - y^m). \tag{2.4}$$

[6] D. Ruelle, Lecture Notes of the Theoretical Physics Institute, University of Colorado, Boulder, Summer 1963.

Furthermore, $e^{-\beta H_m}$ is a bounded operator in $L^2(\Lambda^m)$ with norm $\leq e^{m\beta B}$. The m-particle reduced density matrix is then defined as

$$\rho_\Lambda(x^m, y^m) = \frac{1}{Z_\Lambda} \sum_{s=0}^{\infty} \frac{z^{m+s}}{s!} \int_{\Lambda^s} du^s \times e^{-\beta H_{m+s}}(u^s, x^m; u^s, y^m) \tag{2.5}$$

or

$$\rho_\Lambda(x^m, y^m) = \frac{1}{Z_\Lambda} \sum_{s=0}^{\infty} \frac{z^{m+s}}{s!} \int du^s P_{u^s x^m, u^s y^m}(d\omega^{m+s}) \times \alpha_\Lambda(\omega^{m+s}) \exp[-U_{m+s}(\omega^{m+s})], \tag{2.6}$$

where

$$Z_\Lambda = \sum_{m=0}^{\infty} \frac{z^m}{m!} \int dx^m P_{x^m,x^m}(d\omega^m)\alpha_\Lambda(\omega^m) \times \exp[-U_m(\omega^m)] \tag{2.7}$$

is the grand partition function. (2.6) can be written as

$$\rho_\Lambda(x^m, y^m) = \int P_{x^m,y^m}(d\omega^m, \rho_\Lambda(\omega^m), \tag{2.8}$$

where

$$\rho_\Lambda(\omega^m) = \frac{1}{Z_\Lambda} \sum_{s=0}^{\infty} \frac{z^{m+s}}{s!} \int du^s P_{u^s,u^s}(d\bar{\omega}^s)\alpha_\Lambda(\omega^{m+s}) \times \exp[-U_{m+s}(\omega^{m+s})] \tag{2.9}$$

by use of the Fubini theorem and uniform convergence due to (2.4).

By analogy with the classical case (See Ref. 1), we now define Banach spaces E_ξ as follows. Let E be the complex vector space of sequences of Wiener integrable essentially bounded functionals of m trajectories $\varphi = \varphi(\omega^m)$, where $m = 1, 2, \cdots$. The subspace of those φ's for which

$$||\varphi||_\xi = \sup_m \left[\frac{1}{\xi^m} \text{ess. sup. } |\varphi(\omega^m)|\right] < +\infty \tag{2.10}$$

is a Banach space E_ξ for the norm $||\varphi||_\xi$.

From (2.2) and (2.9) it follows that

$$\begin{aligned} |\rho_\Lambda(\omega^m)| &\leq \frac{1}{|Z_\Lambda|} \sum_{s=0}^{\infty} \frac{|z|^{m+s}}{s!} \exp[(m+s)\beta B] \frac{1}{\lambda^{\nu s}} V^s \\ &\leq [|z|\, e^{\beta B}]^m\, |Z_\Lambda|^{-1} \exp[(V/\lambda^\nu)\, |z|\, e^{\beta B}]. \end{aligned} \tag{2.11}$$

Therefore $\rho_\Lambda = (\rho_\Lambda(\omega^m),\ m = 1, 2, \cdots)$, where the $\rho_\Lambda(\omega^m)$ are defined by (2.9) is a vector in E_ξ for any ξ such that $|z|\, e^{\beta B} \leq \xi$ with norm

$$||\rho_\Lambda||_\xi \leq |Z_\Lambda|^{-1} \exp[(V/\lambda^\nu)\, |z|\, e^{\beta B}]. \tag{2.12}$$

One shows similarly that Z_Λ is an entire function of z and is bounded by

$$|Z_\Lambda| \leq \exp\left[(V/\lambda^\nu)\,|z|\,e^{\beta B}\right]. \tag{2.13}$$

It should be noted that both numerator and denominator in (2.12) $\to \infty$ as exponential functions of V as $V \to \infty$. This indicates the need for such methods as the one used in the following section.

3. INTEGRAL EQUATIONS FOR THE $\rho_\Lambda(\omega^m)$

We first show that the $\rho_\Lambda(\omega^m)$ defined by (2.9) satisfy integral equations similar to the Kirkwood–Salzburg equations.[5] (2.9) can be written as

$$\rho_\Lambda(\omega^m) = \frac{1}{Z_\Lambda}\sum_{s=0}^{\infty}\frac{z^{m+s}}{s!}\int du^s P_{u^s,u^s}(d\tilde\omega^s)\alpha_\Lambda(\omega^{m+s})$$
$$\times \exp\left[-U_{m-1+s}(\omega^{m-1},\tilde\omega^s)\right]\exp\left[-F_1(\omega^m)\right]$$
$$\times \prod_{i=1}^{m}\exp\left[-\int_0^\beta \Phi[\omega_1(t)-\tilde\omega_i(t)]\,dt\right] \tag{3.1}$$

where ω^{m-1} is obtained from ω^m by removing ω_1 and where

$$F_1(\omega^m) = \int_0^\beta \sum_{i=2}^{m}\Phi[\omega_i(t)-\omega_1(t)]\,dt. \tag{3.2}$$

$$\rho_\Lambda(\omega^m) = \frac{1}{Z_\Lambda}\sum_{s=0}^{\infty}\frac{z^{m+s}}{s!}\alpha_\Lambda(\omega_1)\exp\left[-F_1(\omega^m)\right]$$
$$\times \int du^s P_{u^s,u^s}(d\tilde\omega^s)\alpha_\Lambda(\omega^{m-1+s})$$
$$\times \exp\left[-U_{m-1+s}\right]\sum_{n=0}^{s}\frac{s!}{n!\,(s-n)!}K(\omega_1,\tilde\omega^n) \tag{3.3}$$

where

$$K(\omega_1,\tilde\omega^n) = \prod_{i=1}^{n}\left\{\exp\left[-\int_0^\beta \Phi[\omega_1(t)-\tilde\omega_i(t)]\,dt\right]-1\right\}. \tag{3.4}$$

Let $s-n=q$. Then

$$\rho_\Lambda(\omega^m) = Z_\Lambda^{-1}z\alpha_\Lambda(\omega_1)\exp\left[-F_1(\omega^m)\right]$$
$$\times \sum_{n,q=0}^{\infty}\frac{1}{n!}\int du^n P_{u^n,u^n}(d\tilde\omega^n)K(\omega_1,\tilde\omega^n)$$
$$\times \frac{z^{m-1+n+q}}{q!}\int du^q P_{u^q,u^q}(d\tilde\omega^q)\alpha_\Lambda(\omega^{m-1+n+q})$$
$$\times \exp\left[-U_{m-1+n+q}(\omega^{m-1},\tilde\omega^{n+q})\right]. \tag{3.5}$$

Finally we obtain

$$\rho_\Lambda(\omega^m) = \alpha_\Lambda(\omega_1)z\exp\left[-F_1(\omega^m)\right]$$
$$\times\left\{\sum_{n=0}^{\infty}\frac{1}{n!}\int du^n P_{u^n,u^n}(d\tilde\omega^n)K(\omega_1,\tilde\omega^n)\right.$$
$$\left.\times\,\rho_\Lambda(\omega^{m-1},\tilde\omega^n)\right\}\quad\text{for}\quad m>1 \tag{3.6}$$

$$\rho_\Lambda(\omega_1) = \alpha_\Lambda(\omega_1)z\left[1+\sum_{n=1}^{\infty}\frac{1}{n!}\int du^n P_{u^n,u^n}(d\tilde\omega^n)\right.$$
$$\left.\times\,K(\omega_1,\tilde\omega^n)\rho_\Lambda(\tilde\omega^n)\right]. \tag{3.7}$$

The first term in the sum in Eq. (3.6) is simply $\rho(\omega^{m-1})$. The interchange of summations and integrations can be justified by using the bounds of the preceding section.

We next use the fact that $\rho_\Lambda(\omega^m)$ is a symmetric function of the m trajectories ω_i to symmetrize Eq. (3.6) by the same method as in the classical case (see Ref. 1). (2.2) can be written as

$$\sum_{i=1}^{m}F_i(\omega^m) \equiv 2U_m(\omega^m) \geq -2m\beta B, \tag{3.8}$$

where $F_i(\omega^m)$ is defined by analogy with (3.2).

Therefore, for at least one j,

$$F_j(\omega^m) \geq -2\beta B. \tag{3.9}$$

Let W_i^m be the subset of S^m such that $\omega^m \in W_i^m$ implies $F_i(\omega^m) \geq -2\beta B$. (3.9) means that $S^m = \bigcup_{i=1}^m W_i^m$. Let η_i be the characteristic function of W_i^m and $\theta_i = \eta_i/\sum_{i=1}^m \eta_i$. Then $\sum_1^m \theta_i = 1$. Let Π_k be the operator defined on functions of m trajectories $\varphi(\omega^m)$ as the circular permutation of k steps on the arguments of these functions and let Π be the operator defined by

$$\Pi\varphi(\omega^m) = \sum_{k=1}^{m}\Pi_k[\theta_1(\omega^m)\varphi(\omega^m)]. \tag{3.10}$$

If φ is a symmetric function, Π reduces to the identity. Applying Π to both sides of (3.6) gives

$$\rho_\Lambda = A_\Lambda(\zeta + K\rho_\Lambda), \tag{3.11}$$

where $\rho_\Lambda \in E$ is defined in Sec. 2.

ζ is the vector in E defined by $\zeta(\omega_1) = z$, $\zeta(\omega^m) = 0$ $(m>1)$. ζ belongs to E_ξ for any $\xi > 0$ and $\|\zeta\|_\xi = |z|/\xi$.

A_Λ is the linear operator defined by $(A_\Lambda\varphi)(\omega^m) = \alpha_\Lambda(\omega^m)\varphi(\omega^m)$, and is a norm decreasing operator of each E_ξ into itself.

K is the linear operator defined in E by:

$$(K\varphi)(\omega^m) = z\sum_{k=1}^{m}\Pi_k\left\{\theta_1(\omega^m)\exp\left[-F_1(\omega^m)\right]\right.$$
$$\times\left[\sum_{n=0}^{\infty}\frac{1}{n!}\int du^n P_{u^n,u^n}(d\tilde\omega^n)\right.$$
$$\left.\left.\times\,K(\omega_1,\tilde\omega^n)\varphi(\omega^{m-1},\tilde\omega^n)\right]\right\}\quad\text{for}\quad m>1, \tag{3.12}$$

$$(K\varphi)(\omega_1) = z \sum_{n=1}^{\infty} \frac{1}{n!} \int du^n P_{u^n,u^n}(d\bar{\omega}^n) \times K(\omega_1, \bar{\omega}^n)\varphi(\bar{\omega}^n). \quad (3.13)$$

We next show that K is a bounded operator of E_ξ into itself. Let $\varphi \in E_\xi$. From (2.10), (3.4), (3.9), it follows that

$$|K\varphi(\omega^m)| \leq |z|\, ||\varphi||_\xi\, e^{2\beta B}\xi^{m-1} \sum_{n=0}^{\infty} \frac{\xi^n}{n!} [C(\beta)]^n \leq |z|\, ||\varphi||_\xi\, \xi^m \frac{1}{\xi} \exp [2\beta B + \xi C(\beta)], \quad (3.14)$$

where

$$C(\beta) = \sup_\omega \int du P_{uu}(d\bar{\omega}) \times \left| \exp\left[-\int_0^\beta \Phi(\omega(t) - \bar{\omega}(t))\, dt \right] - 1 \right| \quad (3.15)$$

provided $C(\beta) < \infty$. We prove in Appendix 2 that under conditions (a) to (d) on the potential Φ,

$$C(\beta) \leq \bar{C}(\beta) = (1/\lambda^r)\beta e^{2\beta B} \int |\Phi(x)|\, dx. \quad (3.16)$$

Therefore K is a bounded operator in E_ξ with $||K||_\xi \leq |z|\, \xi^{-1} \exp [2\beta B + \xi\bar{C}(\beta)]$. The best bound is obtained for $\xi = [\bar{C}(\beta)]^{-1}$ and is

$$||K||_\xi \leq k = |z|\, \bar{C}(\beta) \exp [2\beta B + 1]. \quad (3.17)$$

Therefore, for any $z \in \Delta$, where

$$\Delta = \{z : |z| < \bar{C}(\beta)^{-1} \exp [-2\beta B - 1]\}, \quad (3.18)$$

Eq. (3.11) has a unique solution in E_ξ; ζ and K are entire (vector-valued) functions of z; therefore the solution is an analytic function of z in Δ. Moreover

$$||\rho_\Lambda||_\xi \leq (|z|/\xi)(1 - k)^{-1} \leq (1 - k)^{-1}. \quad (3.19)$$

It follows from (2.12) and the fact that Z_Λ has no zero on the positive real axis that the solution of (3.11) coincides with ρ_Λ as defined by (2.9) for z real, > 0, and $\in \Delta$. Now we get from Eqs. (2.7) and (2.9),

$$\int \rho_\Lambda(\omega) P_{uu}(d\omega)\, du = z \frac{d}{dz} \log Z_\Lambda. \quad (3.20)$$

The left-hand side is analytic in Δ, and Z_Λ is an entire function [with $Z_\Lambda(0) = 1$]. Therefore Z_Λ has no zeros in Δ and ρ_Λ as defined by (2.9) and (3.11) coincide throughout Δ.

Substituting the solution of (3.11) in (2.8) shows that $\rho_\Lambda(x^m, y^m)$ is an analytic function of z in Δ with values in the space of bounded operators on $L^2(\Lambda^m)$. From (3.19) it follows that

$$|\rho_\Lambda(x^m, y^m)| \leq (1 - k)^{-1}[\bar{C}(\beta)]^{-m}\psi_\beta(x^m - y^m). \quad (3.21)$$

$\psi_\beta(x^m - y^m)$ considered as an operator on $L^2(\Lambda^m)$ is norm-decreasing; therefore

$$||\rho_\Lambda(x^m, y^m)||_2 \leq (1 - k)^{-1}[\bar{C}(\beta)]^{-m}. \quad (3.22)$$

4. LIMIT OF INFINITE VOLUME (CLASSICAL STATISTICS)

The essential point in the preceding argument is that the bound on K is volume independent. Therefore the equation obtained from (3.11) by letting the volume be infinite

$$\rho = \zeta + K\rho \quad (4.1)$$

has a unique solution in E_ξ for $z \in \Delta$, with the same analyticity properties as derived for ρ_Λ. Here we show that $\rho_\Lambda \to \rho$ in some sense as Λ becomes infinite. The method is the same as in the classical case (see Ref. 1).

Let Λ be a sphere with fixed center. This is no loss in generality. We label A, α, and ρ by its radius. Let $\delta' > \delta > 0$. Let $z \in \Delta$. Consider first

$$||A_R K A_{R+\delta'} - A_R K A_{R+\delta}||_\xi.$$

Let $\varphi \in E_\xi$. Then

$$|(A_R K A_{R+\delta'} - A_R K A_{R+\delta})\varphi(\omega^m)| \leq |z|\, e^{2\beta B} \sum_0^\infty \frac{1}{n!} \xi^{m+n-1} \times \alpha_R(\omega_1) \times \int du^n P_{u^n,u^n}(d\bar{\omega}^n)\, |[\alpha_{R+\delta'}(\bar{\omega}^n) - \alpha_{R+\delta}(\bar{\omega}^n)]K(\omega_1, \bar{\omega}^n)|\, ||\varphi||_\xi. \quad (4.2)$$

From

$$|\alpha_{R+\delta'}(\bar{\omega}^n) - \alpha_{R+\delta}(\bar{\omega}^n)| \leq \sum_{i=1}^{n} \alpha_{R+\delta'}(\bar{\omega}_i^{n-1})\, |\alpha_{R+\delta'}(\bar{\omega}_i) - \alpha_{R+\delta}(\bar{\omega}_i)| \quad (4.3)$$

(where $\bar{\omega}_i^{n-1}$ is obtained from $\bar{\omega}^n$ by removing $\bar{\omega}_i$) it follows that the right-hand side of (4.2) is bounded by

$$|z|\, e^{2\beta B} \sum_1^\infty \frac{1}{n!} \xi^{m+n-1} n C(\beta)^{n-1} C_{\delta,R}(\beta)\, ||\varphi||_\xi \quad (4.4)$$

$$= \xi^m\, ||\varphi||_\xi\, |z| \exp [2\beta B + \xi C(\beta)] C_{\delta,R}(\beta), \quad (4.5)$$

where

$$C_{\delta,R}(\beta) = \sup_\omega \int du P_{uu}(d\bar{\omega})\, |K(\omega, \bar{\omega})|. \quad (4.6)$$

It is understood that the trajectory ω lies entirely in Λ_R and the integration is restricted to the con-

tinuous $\tilde{\omega}$ which have at least one point outside $\Lambda_{R+\delta}$. $C_{\delta,R}(\beta)$ is obviously bounded uniformly in R and δ by $C(\beta)$. Furthermore, it is shown in Appendix 2 that:

$$C_{\delta,R}(\beta) \leq \frac{1}{\lambda^{\nu}} \beta e^{2\beta B}\left\{\int_{|x|>\delta/2} |\Phi(x)|\, dx + \int |\Phi(x)|\, dx\, c\sigma(\delta/8, \beta)\right\}. \tag{4.7}$$

This bound depends on δ alone, and not on R. It tends to zero as $\delta \to \infty$. In view of future application to more complicated cases (hard-core potentials) however, we shall make use only of the weaker property: $C_{\delta,R+p\delta}(\beta) \to 0$ as $\delta \to \infty$ for fixed $R > 0$, $p > 0$. From (4.5) and (4.7) ,we obtain:

$$||A_R K A_{R+\delta'} - A_R K A_{R+\delta}||_\xi \leq |z| \times \exp[2\beta B + \xi C(\beta)] C_{\delta,R}(\beta) \leq \eta(\delta, R), \tag{4.8}$$

where $\eta(\delta, R)$ is an increasing function of R, and such that $\eta(\delta, R + p\delta)$ tends to zero as δ tends to infinity for fixed $R > 0$, $p > 0$.

From this we get, as in Ref. 1,

$$||A_R(A_{R+j\delta}K)^i A_{R+j\delta} - A_R K^i||_\xi \leq k^{i-1}\left\{\sum_{i=1}^{j-1} \eta(\delta, R + [i-1]\delta) + \sum_{i=1}^{j} \eta(\delta, R + [i-1]\delta)\right\} \leq 2jk^{i-1}\eta(\delta, R + j\delta). \tag{4.9}$$

From

$$\left\|(1-K)^{-1} - \sum_0^n K^i\right\| \leq \frac{k^{n+1}}{(1-k)} \tag{4.10}$$

and the corresponding relation for $A_{R+\delta}K$, we get by using (4.9), where we replace $j\delta$ by δ:

$$||A_R(1 - A_{R+\delta}K)^{-1}A_{R+\delta} - A_R(1-K)^{-1}||_\xi \leq 2\frac{k^{n+1}}{1-k} + 2\sum_{i=1}^{n} jk^{i-1}\eta\left(\frac{\delta}{j}, R + \delta\right). \tag{4.11}$$

Therefore

$$||A_R\rho_{R+\delta} - A_R\rho||_\xi \leq 2\frac{k^{n+1}}{1-k} + 2\sum_{i=1}^{n} jk^{i-1}\eta\left(\frac{\delta}{j}, R + \delta\right). \tag{4.12}$$

For fixed R, this can be made arbitrarily small by choosing first n and then δ. We have proved:

Lemma 1: Let S_R be the set of continuous trajectories contained in the sphere Λ_R. Then the restriction to S_R of $\rho_{R+\delta}$ tends to the restriction to S_R of ρ as $\delta \to \infty$, in the sense of the E_ξ topology.

Note that in the present case, $\eta(\delta, R)$ is independent of R. Therefore, in the same way as in the classical case,[1] the limit in (4.12) is uniform in R.

We now consider the $\rho(x^m, y^m)$. We prove

Lemma 2: $\rho_h(x^m, y^m)$ tends to $\rho(x^m, y^m)$ uniformly on the compact sets as $h \to \infty$.

Let D be a compact set contained in a sphere Λ_{R-r} of radius $R - r$, and $\delta > 0$. Let

$$||A_R\rho_{R+\delta} - A_R\rho||_\xi \leq \epsilon(\delta, R), \tag{4.13}$$

where $\epsilon(\delta, R) \to 0$ as $\delta \to \infty$ for fixed R. Let x^m, $y^m \in D^m$. Now:

$$|\rho_{R+\delta}(x^m, y^m) - \rho(x^m, y^m)| \leq \int P_{x^m,y^m}(d\omega^m)\, |\rho_{R+\delta}(\omega^m) - \rho(\omega^m)|. \tag{4.14}$$

We split the trajectories into two classes: (α) those which stay in Λ_R^m contribute a term bounded by $\epsilon(\delta, R)\xi^m/\lambda'^m$; ($\beta$) those which have points outside Λ_R^m belong to $K'(r, \beta)$ (A1.5). From (A1.7) it follows that their contribution is bounded by

$$2\,||\rho||_\xi\, \xi^m mc\sigma(r/4, \beta)(1/\lambda'^m).$$

Therefore

$$|\rho_{R+\delta}(x^m, y^m) - \rho(x^m, y^m)| \leq \epsilon(\delta, R)\frac{\xi^m}{\lambda'^m} + 2\,||\rho||_\xi \frac{\xi^m}{\lambda'^m} mc\sigma\left(\frac{r}{4}, \beta\right). \tag{4.15}$$

This can be made arbitrarily small by choosing successively r and δ big enough.

From Lemma 2, the identity for $z \in \Delta$ of the ρ_Δ defined by (2.9) and (3.11), and Lemma 9 in Appendix 1, it follows easily that the $\rho(x^m, y^m)$ are continuous functions of their arguments for any (x^m, y^m) such that none of the $x_i - x_k$, $(j \neq k)$ or $y_i - y_k$ $(j \neq k)$ lies in F.

We next prove the following.

Theorem 1: $\rho_h(x^m, y^m) \to \rho(x^m, y^m)$ in the sense of the strong topology for the operators on $L^2[(R')^m]$.

Consider first $\varphi \in L^2[(R')^m]$ with compact support D_m enclosed in Λ_{R-r}^m where Λ_{R-r} is the sphere of radius $R - r$. Let

$$\Delta\rho(x^m, y^m) = \rho_{R+\delta}(x^m, y^m) - \rho(x^m, y^m) \tag{4.16}$$

$$|\Delta\rho(x^m, y^m)| \leq \epsilon_1(\delta, R) \quad \text{for} \quad x^m \text{ and } y^m \in \Lambda_R^m.$$

Consider

$$||\Delta\rho\varphi||^2 = \int dx^m\, dy^m\, dy'^m \times |\Delta\rho(x^m, y^m)\, \Delta\rho(x^m, y'^m)\varphi(y^m)\varphi(y'^m)|. \tag{4.17}$$

Let V be the volume of Λ_{R-r} and V' the volume of Λ_R. We split the x integration as follows.

(1) $x^m \in \Lambda_R^m$. This region contributes a term $\leq \epsilon_1^2 V'^m V^{2m} ||\varphi||^2$. (4.18)

(2) $x^m \notin \Lambda_R^m$. The contribution of this region is bounded by

$$[2\xi^m ||\rho||_\xi]^2 \int_{x^m \notin \Lambda_R{}^m} dx^m\, dy^m\, dy'^m$$

$$\times \psi_\beta(x^m - y^m)\psi_\beta(x^m - y'^m)\, |\varphi(y^m)\varphi(y'^m)| \quad (4.19)$$

$$\leq [2\xi^m ||\rho||_\xi]^2 m \cdot V^{2m} ||\varphi||^2 (1/\lambda^{r m})\sigma(r, \beta). \quad (4.20)$$

This quantity tends to zero as r (or R) tends to infinity, φ (and therefore V) being held fixed; from (4.18) and (4.20) it follows that $\Delta\rho\varphi \to 0$ in L^2 as $\delta \to \infty$. Therefore $\rho_\Lambda \varphi \to \rho\varphi$ in L^2 for any φ in a dense subset of L^2; from this it follows immediately that $\rho_\Lambda \to \rho$ strongly.

We next turn to the virial expansion.

From translation invariance due to Condition (a) and continuity of $\rho(x, y)$ it follows that $\rho(x, x) = \rho_0$ is a well-defined constant which is an analytic function of z in Δ and is to be interpreted as the analytic continuation of the density. From (2.7)–(2.9) we get

$$\left|\frac{1}{V_{R+\delta}} z \frac{d}{dz} \log Z_{R+\delta} - \rho_0\right|$$

$$\leq \frac{1}{V_{R+\delta}} \int |\rho_{R+\delta}(x, x) - \rho_0|\, \alpha_{R+\delta}(x)\, dx, \quad (4.21)$$

where $V_{R+\delta}$ and $\alpha_{R+\delta}$ are the volume and characteristic function of $\Lambda_{R+\delta}$. From Lemma 2 we get

$$|\rho_{R+\delta}(x, x) - \rho_0|\, \alpha_R(x) \leq \epsilon_1(\delta, R), \quad (4.22)$$

where $\epsilon_1(\delta, R)$ is easily seen to $\to 0$ as $\delta, R \to \infty$ for fixed δ/R. From (4.22) and (3.21) we get

$$\left|\frac{1}{V_{R+\delta}} z \frac{d}{dz} \log Z_{R+\delta} - \rho_0\right|$$

$$\leq \epsilon_1(\delta, R) + \frac{2\xi}{1-k} \frac{1}{\lambda^\nu}\left[1 - \frac{R^\nu}{(R+\delta)^\nu}\right], \quad (4.23)$$

which can be made arbitrarily small by choosing sucessively δ/R and δ. Therefore

$$\lim_{R\to\infty} \frac{z}{V_R} \frac{d}{dz} \log Z_R = \rho_0, \quad (4.24)$$

the convergence being uniform on the compacts in Δ. We have therefore:

Theorem 2: The function $(1/V) \log Z_\Lambda$ is analytic for $z \in \Delta$ and converges uniformly on the compacts as the radius R of Λ becomes infinite.

From this it follows as in Ref. 1 that the virial expansion converges in a neighborhood of the origin.

5. THE REDUCED DENSITY MATRICES (QUANTUM STATISTICS)

We turn to the case of a system which obeys quantum statistics. Throughout this section the potential Φ is supposed to satisfy Conditions (a) → (d) [*not* (d′)]. The system is enclosed in a bounded open region Λ with volume V.

The m particle reduced density matrix is then defined[7] as

$$\rho_\Lambda(x^m, y^m) = \frac{1}{Z_\Lambda} \sum_0^\infty \frac{z^{m+s}}{s!} \int_\Lambda du^s \sum_\Pi (\pm)^\Pi \times e^{-\beta H_{m+s}}[u^s, x^m; \Pi(u^s, y^m)], \quad (5.1)$$

where Π is a permutation of the appropriate number of variables, here $m + s$.

The second sum runs over the elements of the symmetric group S_{m+s}.

$(\pm)^\Pi$ is: $+1$ for Bose statistics
the signature of the permutation Π for Fermi statistics.

Substituting (2.3) into (5.1) gives

$$\rho_\Lambda(x^m, y^m) = \frac{1}{Z_\Lambda} \sum_0^\infty \frac{z^{m+s}}{s!} \int du^s \sum_\Pi (\pm)^\Pi \times P_{u^s, x^m; \Pi(u^s, y^m)}(d\omega^{m+s})\alpha_\Lambda(\omega^{m+s}) \exp[-U_{m+s}(\omega^{m+s})]. \quad (5.2)$$

Z_Λ is the grand partition function

$$Z_\Lambda = \sum_0^\infty \frac{z^m}{m!} \int dx^m \sum_\Pi (\pm)^\Pi P_{x^m, \Pi(x^m)}(d\omega^m)\alpha_\Lambda(\omega^m) \times \exp[-U_m(\omega^m)]. \quad (5.3)$$

We shall now put (5.2) in a more useful form. This involves interchange of summations and integrations. We first forget convergence requirements and perform the algebraic operations. We next give absolute bounds uniform with respect to the integration variables, which justify these operations. (5.2) involves an integration over $(m + s)$ trajectories with s identifications of endpoints. In the case of Maxwell–Boltzmann statistics (hereafter referred to as MB case), this gives m trajectories $x^m \to y^m$ of length (defined as the length of the t interval) β and s closed cycles of length β. Here, due to the permutation Π, there may be μ_i (nonnegative

[7] C. Bloch, *Diagram Expansions in Quantum Statistical Mechanics* (North-Holland Publishing Company, Amsterdam, to be published).

integer) extra trajectories inserted between x_i and the y reached from it (which in general is not y_i) whereas the remaining closed cycles may consist of several trajectories of length β. Let $|\mu| = \sum_1^m \mu_i$. Then

Lemma

$$[\sum_{\Pi} (\pm)^{\Pi}\Pi]P_{u^s,x^m;u^s,y^m}(d\omega^{m+s})\,du^s$$
$$= [\sum_{\Pi} (\pm)^{\Pi}\Pi]_m \sum_{r=0}^{s} C_s^r (\sum_{\Pi} (\pm)^{\Pi}\Pi)_r (s-r)!\,(\pm)^{|\mu|}$$
$$\times \sum_{\mu^m} P_{u^r,u^r}(d\tilde{\omega}^r)\,du^r P^{\mu^m+1}_{x^m,y^m}(d\omega^m),$$

where: the permutation sums labeled m and r operate in an obvious way on the differential elements containing the variables (x^m, y^m) and (u^r, u^r) respectively.

The last summation is understood to be restricted to $|\mu| = s - r$.

The superscript $\mu^m + 1$ in the last factor means that the trajectory $x_i \to y_i$ has length $(\mu_i + 1)\beta$.

In fact, for given $|\mu|$ or r, one has to distribute y^m in all possible ways on the open trajectories starting from x^m (first factor); select out of s variables the r which are not on these open trajectories (second factor); make all permutations of these variables between themselves. There are still $(s - r)!$ ways of distributing the remaining $s - r = |\mu|$ remaining variables on the open trajectories; each of them gives the same contribution. The factor $(\pm)^{|\mu|}$ is easily obtained by induction over $|\mu|$. The interpretation of the lemma in terms of graphs drawn on a cylinder of circumference β, similar to the graphs obtained in perturbation theory[7] is straightforward.

From (5.2) and the preceding lemma, we obtain easily

$$\rho_\Lambda(x^m, y^m) = \sum_{\Pi} (\pm)^{\Pi} \sum_{\mu^m=0}^{\infty} (\pm)^{|\mu|} \times \int P^{\mu^m+1}_{x^m,\Pi(\mu^m)}(d\omega^m)\rho_\Lambda(\omega^m, \mu^m), \tag{5.4}$$

where

$$\rho_\Lambda(\omega^m, \mu^m) = \frac{1}{Z_\Lambda} \sum_{r=0}^{\infty} \frac{z^{m+|\mu|+r}}{r!} \int du^r \sum_{\Pi} (\pm)^{\Pi} \times P_{u^r,\Pi(u^r)}(d\tilde{\omega}^r)\alpha_\Lambda(\omega^m, \tilde{\omega}^r) \exp[-U(\omega^m, \mu^m, \tilde{\omega}^r)]. \tag{5.5}$$

The exponent in the last factor is the same as in (5.2) with only a change in the notation of the variables: $|\mu|$ trajectories have been taken out of s and have been included in ω^m. We shall need the following elementary properties of the symmetric group φ_r. Any permutation Π is a product of cycles. Let γ_j be the number of cycles of length j. $\sum_1^r j\gamma_j = r$. A class γ of conjugate elements consists of those permutations which have the same partition into cycles, i.e., the same γ_j's. The elements in γ are obtained by distributing the r elements in all possible ways in these cycles. Their number is[8]

$$h_\gamma^r = r! \Big/ \prod_{j=1}^{r} [j^{\gamma_j}(\gamma_j!)]. \tag{5.6}$$

Consider now the integration over $\tilde{\omega}^r$, u^r in (5.5). The contribution of $\Pi \in \varphi_r$ depends only on the class γ of Π; two elements in the same γ give contributions which differ only by a relabelling of integration variables. (In terms of graphs, there is a 1–1 correspondence between the classes γ and the unlabeled graphs formed by the $\tilde{\omega}^r$.) With the notation

$$h_\gamma^r\,d\gamma = du^r \sum_{\Pi\in\gamma} (\pm)^{\Pi} P_{u^r,\Pi(u^r)}(d\tilde{\omega}^r), \tag{5.7}$$

(5.5) becomes

$$\rho_\Lambda(\omega^m, \mu^m) = \frac{1}{Z_\Lambda} \sum_{r=0}^{\infty} \frac{z^{m+|\mu|+r}}{r!} \int \sum_{\gamma} h_\gamma^r\,d\gamma\alpha_\Lambda(\omega^m, \tilde{\omega}^r) \times \exp[-U(\omega^m, \mu^m, \tilde{\omega}^r)]. \tag{5.8}$$

We now give upper bounds which justify the preceding algebraic operations. From (2.2) and (5.8) we obtain

$$|\rho_\Lambda(\omega^m, \mu^m)| \le \frac{1}{|Z_\Lambda|} [|z|\,e^{\beta B}]^{m+|\mu|} \times \left\{ \sum_0^{\infty} \frac{(|z|\,e^{\beta B})^r}{r!} \sum_{\gamma} h_\gamma^r \int |d\gamma| \right\} \tag{5.9}$$

$$\le \frac{1}{|Z_\Lambda|} [|z|\,e^{\beta B}]^{m+|\mu|} \sum_r \sum_{\gamma} \prod_i \frac{1}{\gamma_i!} \times \left[\frac{V(|z|\,e^{\beta B})^i}{\lambda^\nu} \frac{1}{j^{\nu/2+1}} \right]^{\gamma_i} \tag{5.10}$$

by use of (5.6) and the relation $r = \sum j\gamma_i$.

This series is absolutely convergent and sums up to

$$|\rho_\Lambda(\omega^m, \mu^m)| \le \frac{1}{|Z_\Lambda|} [|z|\,e^{\beta B}]^{m+|\mu|} \times \exp\left\{ \frac{V}{\lambda^\nu} \sum_{i=1}^{\infty} \frac{(|z|\,e^{\beta B})^i}{j^{\nu/2+1}} \right\} \tag{5.11}$$

provided $|z|\,e^{\beta B} \le 1$. Similarly, from (5.3) we get

$$|Z_\Lambda| \le \exp\left\{ \frac{V}{\lambda^\nu} \sum_{i=1}^{\infty} \frac{(|z|\,e^{\beta B})^i}{j^{\nu/2+1}} \right\}, \tag{5.12}$$

which shows that Z_Λ is an analytic function of z for $|z| < e^{-\beta B}$.

[8] For instance, H. Börner, *Darstellungen von Gruppen* (Springer-Verlag, Berlin, 1955), p. 28.

By analogy with the MB case we define E as the vector space of sequences of Wiener measurable essentially bounded functionals of m trajectories ω^m of respective lengths $(\mu^m + 1)\beta$. Let $\varphi = \varphi(\omega^m, \mu^m)$; $m = 1, \cdots; \mu_i = 0, 1, \cdots$. We define E_ξ as the subspace of those φ for which

$$||\varphi||_\xi = \sup_{m,\mu^m} \frac{1}{\xi^{m+|\mu|}} \times [\text{ess. sup. } |\varphi(\omega^m, \mu^m)|] < +\infty. \quad (5.13)$$

E_ξ is a Banach space with (5.13) as definition of the norm. (5.11) shows that $\rho_\Lambda = \{\rho_\Lambda(\omega^m, \mu^m)\}$ belongs to E_ξ for

$$|z|\, e^{\beta B} \leq \min(\xi, 1) \quad (5.14)$$

with norm

$$||\rho_\Lambda||_\xi \leq \frac{1}{|Z_\Lambda|} \exp\left\{\frac{V}{\lambda^\nu} \sum_{i=1}^{\infty} \frac{(|z|\, e^{\beta B})^i}{j^{\nu/2+1}}\right\}. \quad (5.15)$$

In view of (5.14) we suppose in the following that $\xi \leq 1$. Finally, for $\rho_\Lambda \in E_\xi$ the series (5.4) is absolutely convergent. In fact:

$$|\rho_\Lambda(x^m, y^m)| \leq ||\rho_\Lambda||_\xi\, m!\, \xi^m \prod_{i=1}^{m} \left\{\sum_{\mu_i=0}^{\infty} \frac{\xi^{\mu_i}}{\lambda^\nu (\mu_i + 1)^{\nu/2}}\right\} \quad (5.16)$$

$$\leq ||\rho_\Lambda||_\xi\, m! \left[\frac{1}{\lambda^\nu} \sum_{k=1}^{\infty} \frac{\xi^k}{k^{\nu/2}}\right]^m \quad (5.17)$$

which converges absolutely for $\xi < 1$.

Remark: The preceding quantities are easily computed for free particles ($\Phi = 0$). $\pm$ is $+$ for Bose statistics and $-$ for Fermi statistics. Then

$$Z_\Lambda = \exp\left\{\sum_1^\infty (\pm)^{i-1} \frac{a_i z^i}{j}\right\}, \quad (5.18)$$

where $a_i = \int P^i_{uu}(d\omega)\, du\, \alpha_\Lambda(\omega)$. Careless replacement of a_i by $V/\lambda^\nu j^{\nu/2}$ gives the well-known result[9]

$$\frac{1}{V} \log Z_\Lambda = \frac{1}{\lambda^\nu} \sum_1^\infty (\pm)^{i-1} \frac{z^i}{j^{\nu/2+1}}. \quad (5.19)$$

Furthermore:

$$\rho_\Lambda(\omega^m, \mu^m) = z^{m+|\mu|}. \quad (5.20)$$

$$\rho_\Lambda(x^m, y^m) = \sum_\Pi (\pm)^\Pi \prod_{i=1}^{m} \rho_\Lambda(x_i, y_{\Pi(i)}), \quad (5.21)$$

where

$$\rho_\Lambda(x, y) = \sum_{i=1}^{\infty} (\pm)^{i-1} z^i \int P^i_{xy}(d\omega)\alpha_\Lambda(\omega). \quad (5.22)$$

[9] For instance, K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1963).

This expression makes sense for Λ infinite.

$$\rho(x, y) = \sum_{i=1}^{\infty} (\pm)^{i-1} \frac{z^i}{j^{\nu/2}} \frac{1}{\lambda^\nu} \exp\left[-\frac{|x-y|^2}{j\beta}\right]. \quad (5.23)$$

In particular, for $x = y$, one gets the well-known result[9]:

$$\rho(x, x) = \rho_0 = \frac{1}{\lambda^\nu} \sum_1^\infty (\pm)^{i-1} \frac{z^i}{j^{\nu/2}}. \quad (5.24)$$

6. INTEGRAL EQUATIONS FOR THE $\varrho_\Lambda(\omega^m, \mu^m)$.

We first show that $\rho_\Lambda(\omega^m, \mu^m)$ as defined by (5.8) satisfy integral equations similar to those obtained in Sec. 3. (5.8) can be written as

$$\rho_\Lambda(\omega^m, \mu^m) = \frac{1}{Z_\Lambda} \exp\left[-F_1(\omega^m, \mu^m)\right] \sum_{r=0}^{\infty} \frac{z^{m+|\mu|+r}}{r!} \times \int \sum_\gamma h^r_\gamma\, d\gamma \alpha_\Lambda(\omega^m, \bar\omega^r) \exp\left[-U(\omega^{m-1}, \mu^{m-1}, \bar\omega^r)\right] \times \exp\left\{-\int_0^\beta \sum_{i=0}^{\mu_1} \sum_{k=1}^{r} \Phi[\omega_1(t + j\beta) - \bar\omega_k(t)]\, dt\right\}, \quad (6.1)$$

where ω^{m-1}, μ^{m-1} is obtained from ω^m, μ^m by removing ω_1, μ_1, and where

$$F_1(\omega^m, \mu^m) = \int_0^\beta \sum_{0 \leq j < k \leq \mu_1} \Phi[\omega_1(t + j\beta) - \omega_1(t + k\beta)]\, dt + \int_0^\beta \sum_{j=0}^{\mu_1} \sum_{k=2}^{m} \sum_{j_k=0}^{\mu_k} \Phi[\omega_1(t + j\beta) - \omega_k(t + j_k\beta)]\, dt. \quad (6.2)$$

For a given γ, the $\bar\omega^r$ are distributed in closed loops c corresponding to the cycles $\bar c$ of γ. Let

$$f(c) = \exp\left\{-\int_0^\beta \sum_{j=0}^{\mu_1} \sum_{\bar\omega_k \in c} \Phi[\omega_1(t + j\beta) - \bar\omega_k(t)]\, dt\right\} - 1 \quad (6.3)$$

(i.e., we collect in $f(c)$ the interactions between ω_1 and c). The last factor in (6.1) is then

$$\prod_{c \in \gamma} [f(c) + 1] = \sum_{\gamma' \subset \gamma} K(\omega_1, \mu_1, \gamma'), \quad (6.4)$$

where

$$K(\omega_1, \mu_1, \gamma') = \prod_{c \in \gamma'} f(c) \quad (6.5)$$

is one term in the expansion of the product in the left-hand side of (6.4). Here, the cycles of γ have been split into two families; the product of the cycles in each of them define two classes γ' and γ'' of permutations of r' and r'' variables respectively; one has $\gamma = \gamma'\gamma''$ and $r = r' + r''$ and the

sum in (6.4) runs over all possible γ' obtained in this way. It is easily seen that the same γ' is obtained in $(\prod_i C_{\gamma_i}^{\gamma_i'})$ ways, that $d\gamma = d\gamma' \, d\gamma''$ and that

$$h_\gamma^r \prod_i C_{\gamma_i}^{\gamma_i'} = \frac{r!}{r'! \, r''!} h_{\gamma'}^{r'} h_{\gamma''}^{r''}. \tag{6.6}$$

Substituting the preceding expressions into (6.1) gives

$$\rho_\Lambda(\omega^m, \mu^m) = \frac{1}{Z_\Lambda} z^{1+\mu_1} \exp[-F_1(\omega^m, \mu^m)]$$
$$\times \sum_{r=0}^{\infty} \sum_{r'=0}^{r} \frac{z^{m-1+|\mu'|+r'+r''}}{r'! \, r''!} \int \sum_{\gamma'} h_{\gamma'}^{r'} \, d\gamma' K(\omega_1, \mu_1, \gamma')$$
$$\times \int \sum_{\gamma''} h_{\gamma''}^{r''} \, d\gamma'' \alpha_\Lambda(\omega^m, \bar{\omega}^r) \exp[-U(\omega^{m-1}, \mu^{m-1}, \bar{\omega}^r)] \tag{6.7}$$

where $|\mu'| = |\mu| - \mu_1$. The sum over r'', γ'' can be performed, due to uniform absolute convergence resulting from the preceding bounds, and introduces again ρ_Λ in the right-hand side. We drop the prime on γ', r' and obtain

$$\rho_\Lambda(\omega^m, \mu^m)$$
$$= \alpha_\Lambda(\omega_1) z^{1+\mu_1} \exp[-F_1(\omega^m, \mu^m)] \sum_{r=0}^{\infty} \frac{1}{r!} \int \sum_{\gamma} d\gamma h_\gamma^r$$
$$\times K(\omega_1, \mu_1, \gamma) \rho_\Lambda(\omega^{m-1}, \mu^{m-1}, \gamma) \quad \text{for} \quad m > 1 \tag{6.8}$$

and similarly

$$\rho_\Lambda(\omega_1, \mu_1) = \alpha_\Lambda(\omega_1) z^{1+\mu_1} \exp[-F_1(\omega_1, \mu_1)]$$
$$\times \left[1 + \sum_{r=1}^{\infty} \frac{1}{r!} \int \sum_{\gamma} d\gamma h_\gamma^r K(\omega_1, \mu_1, \gamma) \rho_\Lambda(\gamma) \right], \tag{6.9}$$

where the argument γ in ρ_Λ represent the family of closed loops c associated with the cycles $\bar{c}$ of the class of permutations γ. In (6.8), $\alpha_\Lambda(\omega_1)$ can be replaced by $\alpha_\Lambda(\omega^m)$.

From now on, we restrict ourselves to purely repulsive potentials [Condition (d')]. Equations (6.8) and (6.9) can be written as

$$\rho_\Lambda = A_\Lambda(\zeta + K\rho_\Lambda), \tag{6.10}$$

where $\rho_\Lambda \in E$ is defined in Sec. 5. ζ is the vector in E defined by

$$\begin{cases} \zeta(\omega_1, \mu_1) = z^{1+\mu_1} e^{-F_1(\omega_1, \mu_1)} \\ \zeta(\omega^m, \mu^m) = 0 \quad \text{for} \quad m > 1; \end{cases} \tag{6.11}$$

ζ belongs to E_ξ for $|z| \leq \xi$, and $||\zeta||_\xi \leq 1$; A_Λ is the linear operator defined by

$$A_\Lambda \varphi(\omega^m, \mu^m) = \alpha_\Lambda(\omega^m) \varphi(\omega^m, \mu^m) \tag{6.12}$$

and is a norm decreasing operator of each E_ξ into itself. K is the linear operator in E defined by

$$K\varphi(\omega^m, \mu^m) = z^{1+\mu_1} \exp[-F_1(\omega^m, \mu^m)]$$
$$\times \sum_{r=0}^{\infty} \frac{1}{r!} \int \sum_{\gamma} h_\gamma^r \, d\gamma K(\omega_1, \mu_1, \gamma)$$
$$\times \varphi(\omega^{m-1}, \mu^{m-1}, \gamma) \quad \text{for} \quad m > 1, \tag{6.13}$$

$$K\varphi(\omega_1, \mu_1) = z^{1+\mu_1} \exp[-F_1(\omega_1, \mu_1)]$$
$$\times \sum_{r=1}^{\infty} \frac{1}{r!} \int \sum_{\gamma} h_\gamma^r \, d\gamma K(\omega_1, \mu_1, \gamma) \varphi(\gamma). \tag{6.14}$$

We next show that K is a bounded operator of E_ξ into itself. In fact, let $\varphi \in E_\xi$.

$$|K\varphi(\omega^m, \mu^m)| \leq |z|^{1+\mu_1} [\exp(-F_1)] \, ||\varphi||_\xi \, \xi^{m-1+|\mu'|}$$
$$\times \sum_{r=0}^{\infty} \frac{\xi^r}{r!} \int \sum_{\gamma} h_\gamma^r \, |d\gamma| \, K(\omega_1, \mu_1, \gamma). \tag{6.15}$$

Let $\gamma = \{\gamma_i\}$, let c_i be a loop of length j, and dc_i be defined in an obvious way and such that $|d\gamma| = \prod_i (dc_i)^{\gamma_i}$. (6.5) can be written as

$$K(\omega_1, \mu_1, \gamma) = \prod_j [f(c_j)]^{\gamma_j}. \tag{6.16}$$

Then

$$|K\varphi(\omega^m, \mu^m)| \leq |z|^{1+\mu_1} \, ||\varphi||_\xi \, \xi^{m-1+|\mu'|}$$
$$\times \prod_{j=1}^{\infty} \sum_{\gamma_j=0}^{\infty} \frac{1}{\gamma_j!} \left\{ \frac{\xi^j}{j} \int dc_j \, |f(c_j)| \right\}^{\gamma_j} \tag{6.17}$$
$$\leq |z|^{1+\mu_1} \, ||\varphi||_\xi \, \xi^{m-1+|\mu'|} \exp\left(\sum_{j=1}^{\infty} b_j \frac{\xi^j}{j} \right), \tag{6.18}$$

provided $b_j = \sup_{\omega_1} \int dc_j \, |f(c_j)|$ be finite and such that the series in the exponent be absolutely convergent. We prove in Appendix 2 that under Conditions (a)–(d'),

$$b_j \leq \frac{1}{\lambda^\nu j^{\nu/2}} \beta j(\mu_1 + 1) \int |\Phi(x)| \, dx. \tag{6.19}$$

Therefore

$$|K\varphi(\omega^m, \mu^m)|$$
$$\leq [|z| \exp D(\beta, \xi)]^{1+\mu_1} \xi^{m-1+|\mu'|} \, ||\varphi||_\xi, \tag{6.20}$$

where

$$D(\beta, \xi) = \frac{1}{\lambda^\nu} \beta \int |\Phi| \, dx \sum_1^{\infty} \frac{\xi^j}{j^{\nu/2}}. \tag{6.21}$$

K is a bounded operator in E_ξ for $|z| \leq \xi \exp[-D(\beta, \xi)]$ with norm

$$||K||_\xi \leq |z| \frac{1}{\xi} \exp D(\beta, \xi) = k. \tag{6.22}$$

Let

$$\Delta = \{z : |z| < \xi \exp[-D(\beta, \xi)]\}. \tag{6.23}$$

For any $z \in \Delta$, (6.10) has a unique solution in E_ξ. ζ and K being entire functions of z, this solution is analytic for $z \in \Delta$. Moreover

$$||\rho_\Lambda||_\xi \leq (1-k)^{-1}. \tag{6.24}$$

The same argument as in the MB case shows that ρ_Λ as defined by (5.8) and by (6.10) coincide throughout Δ, and that Z_Λ has no zeros in Δ. Substituting in (5.4) the solution of (6.10) shows that $\rho_\Lambda(x^m, y^m)$ is an analytic function of z in Δ with values in the space of bounded operators on $L^2(\Lambda^m)$. Furthermore

$$||\rho_\Lambda(x^m, y^m)||_2 \leq (1-k)^{-1} m!\, \xi^m (1-\xi)^{-1}.$$

7. LIMIT OF INFINITE VOLUME (QUANTUM STATISTICS)

The argument is the same as in the MB case and we give only the modifications needed in the proof. The first problem is to find an upper bound for

$$||A_R K A_{R+\delta'} - A_R K A_{R+\delta}||_\xi.$$

Let $\varphi \in E_\xi$.

$$\begin{aligned}|(A_R K A_{R+\delta'} - A_R K A_{R+\delta})\varphi(\omega^m, \mu^m)| &\leq |z|^{1+\mu_1}\, ||\varphi||_\xi\, \xi^{m-1+|\mu'|} \\ &\times \exp\left(\sum_1^\infty b_i \frac{\xi^i}{j}\right) \sum_1^\infty \frac{\xi^i}{j} \Delta b_i, \end{aligned} \tag{7.1}$$

where Δb_i is obtained from b_i by restriction of the integration to the loops which have points outside $\Lambda_{R+\delta}$, ω_1 being entirely contained in Λ_R. It is shown in Appendix 2 that

$$\begin{aligned}\sum_1^\infty \Delta b_i \frac{\xi^i}{j} &\leq (\mu_1 + 1)\frac{\beta}{\lambda^\nu}\left\{\int_{|x|>\delta/2} |\Phi(x)|\, dx \sum_1^\infty \frac{\xi^i}{j^{\nu/2}}\right. \\ &\left. + c\int |\Phi(x)|\, dx \sum_1^\infty \frac{\xi^i}{j^{\nu/2}}\, \sigma(\delta/8, j\beta)\right\}, \end{aligned} \tag{7.2}$$

which tends to zero as δ tends to infinity. Therefore

$$\begin{aligned}&||A_R K A_{R+\delta'} - A_R K A_{R+\delta}||_\xi \\ &\leq (\xi/e)\{\xi - |z|\exp[D(\beta, \xi)]\}^{-1}(\beta/\lambda^\nu) \\ &\times \left\{\int_{|x|>\delta/2} |\phi(x)|\, dx \sum_1^\infty \frac{\xi^i}{j^{\nu/2}}\right. \\ &\left. + \int |\phi(x)|\, dx \sum_1^\infty \frac{\xi^i}{j^{\nu/2}}\, \sigma(\delta/8, j\beta)\right\} = \eta(\delta, R), \end{aligned} \tag{7.3}$$

where $\eta(\delta, R)$ has the same properties as in the MB case. Lemma 1 and its proof then hold without change.

Lemma 2 holds without change, the proof being modified as follows. From (5.4) we obtain

$$\begin{aligned}&|\rho_{R+\delta}(x^m, y^m) - \rho(x^m, y^m)| \\ &\leq m! \sup_{x^m, y^m \in D^m} \sum_{\mu^m=0}^\infty \int P^{\mu^m+1}_{x^m y^m}(d\omega^m) \\ &\times |\rho_{R+\delta}(\omega^m, \mu^m) - \rho(\omega^m, \mu^m)|. \end{aligned} \tag{7.4}$$

The contributions of the trajectories of classes (α) and (β) are bounded respectively by

$$m!\, \epsilon(\delta, R)\left[\frac{1}{\lambda^\nu}\sum \frac{\xi^i}{j^{\nu/2}}\right]^m \tag{7.5}$$

and

$$\begin{aligned}m!\, 2\, ||\rho||_\xi\, m\left[\frac{1}{\lambda^\nu}\sum \frac{\xi^i}{j^{\nu/2}}\right]^m \frac{c}{\lambda^\nu} \\ \times\left[\sum_1^\infty \frac{\xi^i}{j^{\nu/2}}\, \sigma\left(\frac{r}{4}, j\beta\right)\right]. \end{aligned} \tag{7.6}$$

The series in the last factor converges uniformly in r and $\to 0$ as $r \to \infty$. The result follows as in the MB case.

Theorem 1 holds with the following change in the proof. The contribution of the region $x^m \notin \Lambda_R^m$ is bounded by

$$\begin{aligned}&[2\, ||\rho||_\xi\, m!]^2 V^{2m}\, ||\varphi||^2 \sup_{y^m, y'^m \in D^m} \int_{x^m \in \Lambda_r{}^m} dx^m \\ &\times\left[\sum_{\mu^m=0}^\infty \xi^{m+|\mu|} P^{\mu^m+1}_{x^m, y^m}(d\omega^m)\right] \\ &\times\left[\sum_{\mu^m=0}^\infty \xi^{m+|\mu|} P^{\mu^m+1}_{x^m, y'^m}(d\omega^m)\right] \end{aligned} \tag{7.7}$$

$$\begin{aligned}&\leq [2\, ||\rho||_\xi\, m!]^2 V^{2m}\, ||\varphi||^2\, m(1-\xi)^{-(m-1)} \\ &\times\left[\frac{1}{\lambda^\nu}\sum_1^\infty \frac{\xi^i}{j^{\nu/2}}\right]^m\left[\sum_1^\infty \xi^i \sigma(r, j\beta)\right]. \end{aligned} \tag{7.8}$$

The last series is uniformly convergent with respect to r and tends to zero as r tends to infinity. Therefore the bound (7.8) tends to zero as r tends to infinity for fixed φ.

The theorem follows as in the MB case. Theorem 2 and the convergence of the virial expansion hold without modification. In the proof, the basic inequality (4.23) is to be replaced by

$$\begin{aligned}\left|\frac{1}{V_{R+\delta}} z\frac{d}{dz}\log Z_{R+\delta} - \rho_0\right| &\leq \epsilon_1(\delta, R) + \frac{2}{1-k}\frac{1}{\lambda^\nu} \\ &\times \sum_{i=1}^\infty \frac{\xi^i}{j^{\nu/2}}\left(1 - \frac{R^\nu}{(R+\delta)^\nu}\right) \end{aligned} \tag{7.9}$$

and $\epsilon_1(\delta, R)$ is easily seen to tend to zero as δ tends to infinity for fixed δ/R, as in the MB case.

8. CONCLUSION.

The main results of our investigation are the following.

(1) The m-particle reduced density matrices, for quantum gases obeying MB (or quantum) statistics, for finite volume $\rho_\Lambda(x^m, y^m)$ and for infinite volume $\rho(x^m, y^m)$ are analytic functions of the activity in a domain Δ defined by (3.18) [or (6.23)] with values in the space of bounded operators on $L^2[(R^r)^m]$.

(2) $\rho(x^m, y^m)$ is the limit of $\rho_\Lambda(x^m, y^m)$ as Λ becomes infinite in the sense of Lemmas 1 and 2 and Theorem 1 of Sec. 4.

(3) The pressure can be continued as an analytic function of z in Δ and the virial expansion converges in a neighborhood of the origin.

The two-body potential Φ is supposed to satisfy Conditions (a) $\rightarrow$ (d) in all cases. In addition, in the case of quantum statistics, we had to impose the very restrictive condition that Φ be > 0, i.e., purely repulsive, [this is needed to ensure the convergence of (6.18) for every μ_1 when b_l is replaced by the bound (A2.10)] and our next task will be to get rid of it.

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APPENDIX 1

Conditional Wiener Measure

We follow closely Ref. 4 (referred to as N). We call x, y, u, v points in l-dimensional Euclidian space R^l. Let

$$\psi_\beta(x - y) = (\pi\beta)^{-l/2} \exp[-(x - y)^2/\beta] \qquad \text{(A1.1)}$$

(in N's notations, we have taken $4D = 1$).

A trajectory ω is a function from the closed interval $[0, \beta]$ into the one point compactification $\dot{R}^l$ of R^l. The trajectories form a space

$$\Omega = \coprod_{0 \le t \le \beta} \dot{R}^l$$

which is compact for the topology of pointwise convergence.

The conditional Wiener measure is defined on the continuous functionals of the type $f(\omega) = F[\omega(t_1), \cdots, \omega(t_n)]$, where $0 < t_1 < \cdots < t_n < \beta$, and where F is a continuous function of n points of $\dot{R}^l$, by

$$P_{xy}(f) = \int \psi_{t_1}(x_1 - x)\psi_{t_2 - t_1}(x_2 - x_1) \cdots \times \psi_{\beta - t_n}(y - x_n)\, dx_1 \cdots dx_n F(x_1, \cdots, x_n) \qquad \text{(A1.2)}$$

and extended to the class $\mathcal{C}(\Omega)$ of continuous functions on Ω as in N. There exists then a regular measure also denoted P_{xy} such that for all $f \in \mathcal{C}(\Omega)$, $P_{xy}(f) = \int P_{xy}(d\omega)\, f(\omega)$.

Continuity of the Trajectories

Let

$$\sigma(\epsilon, \delta) = \sup_{t \le \delta} \int_{|y - x| > \epsilon} \psi_t(x - y)\, dy \qquad \text{(A1.3)}$$

$$= \frac{\Omega_l}{\pi^{l/2}} \int_{u > \epsilon/(\delta)^{\frac{1}{2}}} e^{-u^2} u^{l-1}\, du, \qquad \text{(A1.4)}$$

where Ω_l is the area of the unit sphere in l-dimensional space. $\sigma(\epsilon, \delta)$ is a function of ϵ^2/δ and $\rightarrow 0$ faster than any power of ϵ^2/δ as $\epsilon^2/\delta \rightarrow \infty$. We now prove

Theorem 1: The measure P_{xy} is concentrated on the ω continuous from $[0, \beta]$ to R^l.

The proof is the same as in N, and we give only the minor modifications needed.

Lemmas 1, 2, 3 hold with the following two changes. The sets A, B, C, D are defined with the additional restriction that all the values of t involved belong to the closed interval $[0, \gamma]$ where γ is fixed, $0 < \gamma < \beta$. The conditional measure of these sets involves an extra factor $\psi_{\beta - t}(y - u)$ where $0 \le t \le \gamma$; this factor is bounded by $[\pi(\beta - \gamma)]^{-l/2}$.

Therefore we get the following result, corresponding in N to

Lemma 3: Let $0 \le a \le b \le \gamma$, with $b - a \le \delta$. Let $E(a, b, \epsilon) = \{\omega : |\omega(t) - \omega(s)| > 2\epsilon$ for some t and s in [a, b]$\}$. Then

$$P_{xy}[E(a, b, \epsilon)] \le 2[\pi(\beta - \gamma)]^{-l/2} \sigma(\tfrac{1}{2}\epsilon, \delta).$$

We suppose to avoid minor complications that γ/δ is an integer. Then we have

Lemma 4: Let

$$F(\gamma, \epsilon, \delta) = \{\omega : |\omega(t) - \omega(s)| > \epsilon \text{ for some } t \text{ and } s \text{ in } [0, \gamma] \text{ with } |t - s| \le \delta\}.$$

Then

$$P_{xy}[F(\gamma, \epsilon, \delta)] \le (2\gamma/\delta)[\pi(\beta - \gamma)]^{-l/2} \sigma(\tfrac{1}{4}\epsilon, \delta).$$

Same proof as in N.

The measure P_{xy} is unchanged by exchange of x and y and reversing the sense of the trajectories. Therefore, γ' being any fixed number in $[0, \gamma]$, we have

Lemma 5: Let

$$G(\gamma', \epsilon, \delta) = \{\omega : |\omega(t) - \omega(s)| > \epsilon \quad \text{for some } t \text{ and } s \text{ in } [\gamma', \beta] \text{ with } |t - s| \leq \delta\}.$$

Then

$$P_{xy}[G(\gamma', \epsilon, \delta)] \leq [2(\beta - \gamma')/\delta](\pi\gamma')^{-l/2}\sigma(\tfrac{1}{4}\epsilon, \delta).$$

Now let

$$K'(\epsilon, \delta) = F(\gamma, \epsilon, \delta) \cup G(\gamma', \epsilon, \delta)$$

or equivalently

$$K'(\epsilon, \delta) = \{\omega : |\omega(t) - \omega(s)| > \epsilon \quad \text{for some } t \text{ and } s \text{ in } [0, \beta] \quad \text{with} \quad |t - s| \leq \delta\}. \tag{A1.5}$$

Then

$$P_{xy}[K'(\epsilon, \delta)] \leq \frac{2}{\delta}\sigma\left(\frac{\epsilon}{4}, \delta\right)\left\{\frac{\gamma}{[\pi(\beta - \gamma)]^{l/2}} + \frac{\beta - \gamma'}{(\pi\gamma')^{l/2}}\right\}. \tag{A1.6}$$

Taking $\gamma = \gamma' = \beta/2$, we get

Lemma 6:

$$P_{xy}[K'(\epsilon, \delta)] \leq c\lambda^{-l}(\beta/\delta)\sigma(\tfrac{1}{4}\epsilon, \delta) \tag{A1.7}$$

with $\lambda = (\Pi\beta)^{\frac{1}{2}}$ and $c = 2^{l/2+1}$.

We now prove Theorem 1. Let S be the set of all continuous trajectories ω. Then

$$S = \bigcap_{\epsilon} \bigcup_{\delta} K(\epsilon, \delta)$$

or

$$S' = \bigcup_{\epsilon} \bigcap_{\delta} K'(\epsilon, \delta)$$

(where for any $X \subset \Omega$, X' means the complement of X). Therefore $P_{xy}(S') = 0$, by Lemma 6.

It can be proved in a similar way that P_{xy} is concentrated on the subset of S consisting of those ω's for which $\omega(0) = x$ and $\omega(\beta) = y$.

Exclusion of a Set of Capacity 0.

The (Newtonian) capacity is defined in Ref. 10. We have the following theorem

Theorem 2: Let F be a closed subset of R^l of capacity 0, and let $x \notin F$, $y \notin F$. Then

$$P_{xy}(\{\omega : \omega(t) \in F \quad \text{for some} \quad t \in [0, \beta]\}) = 0.$$

This is the analogue of Theorem 5 in N and is easily deduced from it. In fact, define, for each pair γ_1, γ_2: $0 \leq \gamma_1 \leq \gamma_2 \leq \beta$.

$$H(\gamma_1, \gamma_2) = \{\omega : \omega(t) \in F \quad \text{for some} \quad t \in [\gamma_1, \gamma_2]\}.$$

Let $0 < \gamma' < \gamma < \beta$. Then

$$H(0, \beta) \subset H(0, \gamma) \cup H(\gamma', \beta).$$

Therefore

$$P_{xy}[H(0, \beta)] \leq P_{xy}[H(0, \gamma)] + P_{xy}[H(\gamma', \beta)] \leq \frac{1}{[\pi(\beta - \gamma)]^{l/2}} \int P_{xu}[H(0, \gamma)]\, du + \frac{1}{(\pi\gamma')^{l/2}} \int P_{vy}[H(\gamma', \beta)]\, dv = 0 \text{ by application of Theorem 5 in N.}$$

Restrictions on the Volume

We have to consider physical systems for which the position x is confined to an open (connected) subset Λ of R^l, and restrict the integration to trajectories which stay in Λ. Let:

$$\Lambda_t = \{\omega : \omega(t) \in \Lambda\}.$$

$$\Omega_\Lambda = \bigcap_{0 \leq t \leq \beta} \Lambda_t$$

$$S_\Lambda = \Omega_\Lambda \cap S.$$

We next prove

Lemma 7: S_Λ is measurable.

S' is measurable (with measure 0), therefore S is measurable. Λ_t is open in Ω, therefore measurable. Let $\mathfrak{D}$ be a dense denumerable subset of $[0, \beta]$. Then, due to continuity,

$$S_\Lambda = (\bigcap_{0 \leq t \leq \beta} \Lambda_t) \cap S = (\bigcap_{t \in \mathfrak{D}} \Lambda_t) \cap S.$$

S_Λ is a denumerable intersection of measurable sets, therefore measurable.

Functional Integral Representation of $\exp[-\beta H]$

(H will be the Hamiltonian for the Schrödinger equation in l dimensions with potential U.) Let $U(x)$ be a real function, bounded from below by $-M$, and continuous in a bounded open connected region Λ, except possibly on a closed set F of capacity zero. Let $\alpha_\Lambda(\omega)$ be the characteristic function of S_Λ. Let

$$f(\omega) = \exp\left\{-\int_0^\beta U[\omega(t)]\, dt\right\}. \tag{A1.8}$$

Then:

Lemma 8: $f(\omega)$ is integrable with respect to $P_{xy}(d\omega)$, for $x \in \Lambda$, $y \in \Lambda$.

The proof is the same as in N. The sequence of

[10] H. Cartan, Bull. Soc. Math. France **73**, 74 (1945).

integrable functionals

$$f_n(\omega) = \exp\left\{-\frac{\beta}{n}\sum_1^n U\left[\omega\left(j\frac{\beta}{n}\right)\right]\right\}$$

converges almost everywhere to $f(\omega)$ and is bounded by the integrable constant functional $e^{\beta M}$. Therefore, by Lebesgue's bounded convergence theorem[11] $f(\omega)$ is integrable and

$$\int f(\omega)P_{xy}(d\omega) \leq e^{\beta M}\psi_\beta(x-y).$$

Lemma 9: $\int P_{xy}(d\omega)\, f(\omega)\, \alpha_\Lambda(\omega)$ is a continuous function of (x, y) for x and $y \in \Lambda - F$.

We first prove the continuity with respect to y. Let $y \in \Lambda - F$, $y' \in \Lambda - F$, $|y - y'| = 2\epsilon$. Let Σ be the sphere of radius $r + \epsilon$ with center at $\frac{1}{2}(y + y')$. ϵ and r are taken small enough so that $\Sigma \subset \Lambda - F$. Let

$$f_\gamma(\omega) = \exp\left\{-\int_0^\gamma U[\omega(t)]\,dt\right\} \qquad \text{(A1.9)}$$

$$|f_\gamma(\omega) - C| \leq \eta \quad \text{for} \quad \omega \subset \Sigma,$$

where $C = \exp[-\gamma U(y)]$. U is continuous at y, therefore η can be made arbitrarily small by taking ϵ and r small enough.

Let $\chi(\omega)$ be the characteristic function of $K(r, \gamma)$ defined in Appendix 1 as the complement of $K'(r, \gamma)$ (A1.5). Let:

$$g(u) = \int P_{xu}^{\beta-\gamma}(d\omega) f_{\beta-\gamma}(\omega)\alpha_\Lambda(\omega). \qquad \text{(A1.10)}$$

(The subscript $\beta - \gamma$ is the length of the t interval.) We have

$$g(u) \leq e^{(\beta-\gamma)M}\psi_{\beta-\gamma}(x-u). \qquad \text{(A1.11)}$$

Then

$$\left|\int [P_{xy}(d\omega) - P_{xy'}(d\omega)]f(\omega)\alpha_\Lambda(\omega)\right|$$

$$= \left|\int g(u)\,du \int [P_{uv}^\gamma(d\omega) - P_{uv'}^\gamma(d\omega)]f_\gamma(\omega)\alpha_\Lambda(\omega)\right|$$

$$\leq \int g(u)\,du C\,|\psi_\gamma(u-y) - \psi_\gamma(u-y')|$$

$$+ \int g(u)\,du \int [P_{uv}^\gamma(d\omega) + P_{uv'}^\gamma(d\omega)]$$

$$\times \{\eta\chi(\omega) + e^{\gamma M}[1-\chi(\omega)]\alpha_\Lambda(\omega) + e^{\gamma M}[1-\alpha_\Lambda(\omega)]\}$$

$$\leq e^{\beta M}\{\epsilon(2/\gamma)[\pi(\beta-\gamma)]^{-l/2}\int du[\psi_\gamma(u-y)$$

$$+ \psi_\gamma(u-y')]\,|2u - y - y'|$$

$$+ \eta[\psi_\beta(x-y) + \psi_\beta(x-y')] + 4c(\pi\gamma)^{-l/2}\sigma(\tfrac{1}{4}r, \gamma)\Big\}$$

by Lemma 6. This can be made arbitrarily small by choosing successively η (i.e., $r + \epsilon$), γ, and ϵ.

It is then straightforward to extend the preceding argument to a proof of the simultaneous continuity in (x, y).

We next define for any $\varphi \in L^2(\Lambda)$

$$T_\beta\varphi(x) = \int P_{xv}(d\omega)f(\omega)\alpha_\Lambda(\omega)\varphi(y)\,dy. \qquad \text{(A1.12)}$$

T_β has the following properties [see N, and also Ref. 12]: T_β is a bounded operator in $L^2(\Lambda)$, with $\|T_\beta\| \leq e^{\beta M}$; $T_\alpha \cdot T_\beta = T_{\alpha+b}$ $(\alpha > 0,\ \beta > 0)$; $\lim_{\beta\to 0} T_\beta\varphi = \varphi$ for all $\varphi \in L^2(\Lambda)$.

Therefore, T_β is a strongly continuous semigroup.[13] Furthermore, T_β is self-adjoint for any $\beta \geq 0$. It then follows[13] that there exists a self-adjoint operator H defined by

$$H = -\lim_{\beta\to 0}(1/\beta)(T_\beta - 1) \qquad \text{(A1.13)}$$

(the limit being in the sense of the strong operator topology), such that $T_\beta = e^{-\beta H}$. It is easily seen, as in N, that for any $\varphi \in L^2(\Lambda)$ which is twice continuously differentiable and has compact support,

$$H\varphi = (-\tfrac{1}{4}\Delta + U)\varphi. \qquad \text{(A1.14)}$$

Therefore, H is a self-adjoint extension of the symmetric operator $-\frac{1}{4}\Delta + U$, and can be taken as the Hamiltonian of a particle in l-dimensional space, with mass $m = 2$ and potential energy U.

APPENDIX 2

Here we prove the various bounds used in the text.

Bound for

$$C(\beta) = \sup_\omega \int f(\bar\omega)P_{uu}(d\bar\omega)\,du \qquad \text{(A2.1)}$$

where

$$f(\bar\omega) = \left|\exp\left[-\int_0^\beta \Phi(\omega(t) - \bar\omega(t))\,dt\right] - 1\right| \qquad \text{(A2.2)}$$

Φ is bounded from below by $2B$. Therefore

$$f(\bar\omega) \leq e^{2\beta B}\int_0^\beta |\Phi(\omega(t) - \bar\omega(t))|\,dt. \qquad \text{(A2.3)}$$

Let $\bar\omega'$ be the trajectory obtained from $\bar\omega$ by applying the translation $-u$. We use the notation: $\bar\omega = \bar\omega' + u$. Then:

[11] P. R. Halmos, *Measure Theory* (D. Van Nostrand Company, Inc., New York, 1950).

[12] E. Nelson, Coll. Intern. CNRS **117**, Paris, 1962.

[13] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Fredrick Ungar Publishing Company, New York, 1955).

$$C(\beta) \leq \sup_{\omega} e^{2\beta B} \int P_{00}(d\tilde{\omega}')\, du \times \int_0^\beta |\Phi(\omega(t) - \tilde{\omega}'(t) - u)|\, dt. \quad \text{(A2.4)}$$

By the Fubini theorem, we can perform successively the integrations on u, on t and on $\tilde{\omega}'$. All three are trivial and we get

$$C(\beta) \leq \bar{C}(\beta), \quad \text{(A2.5)}$$

where

$$\bar{C}(\beta) = \frac{1}{\lambda^\nu} \beta e^{2\beta B} \int |\Phi(x)|\, dx. \quad \text{(A2.6)}$$

In (A2.3), one can replace $e^{2\beta B}$ by $e^{2\beta B - 1}/2\beta B$. One gets then the slightly better bound

$$C(\beta) \leq \frac{e^{2\beta B} - 1}{2B} \frac{1}{\lambda^\nu} \int |\Phi|\, dx. \quad \text{(A2.7)}$$

The improvement in the subsequent applications is negligible.

Upper Bound for b_j (Sec. 6)

The same argument applied to b_j gives a bound which is obtained from $C(\beta)$ by replacing β by $j\beta$ and Φ by $(\mu_1 + 1)\Phi$. Therefore

$$b_j \leq (\lambda^\nu j^{\nu/2})^{-1} \beta j (1 + \mu_1) \times \exp[2j(\mu_1 + 1)\beta B] \int |\Phi(x)|\, dx \quad \text{(A2.8)}$$

which under Condition (d'), i.e., $B = 0$, reduces to (6.19).

Upper Bound for $C_{\delta,R}(\beta)$ as Defined by (4–6) and the Subsequent Restrictions

The domain of the $\tilde{\omega}$ integration is split into two parts.

(1) The $\tilde{\omega}$ which stay entirely outside $\Lambda_{R+\delta/2}$. The same argument as above shows that they contribute a term bounded by

$$\lambda^{-\nu} \beta e^{2\beta B} \sup_{x \in \Lambda_R} \int_{x \in \Lambda_{R+\delta/2}} |\Phi(x - \tilde{x})|\, d\tilde{x} \leq \lambda^{-\nu} \beta e^{2\beta B} \int_{|x| > \delta/2} |\Phi(x)|\, dx. \quad \text{(A2.9)}$$

(2) The $\tilde{\omega}$ which have points inside $\Lambda_{R+\delta/2}$. We replace this restriction by the weaker one: $\tilde{\omega} \in K'(\delta/2, \beta)$ (A1.5). The contribution of these trajectories is bounded by

$$\beta e^{2\beta B} \int |\phi(x)|\, dx \int_{K'(\delta/2,\beta)} P_{00}(d\tilde{\omega}) \quad \text{(A2.10)}$$

$$\leq \beta e^{2\beta B} \int |\phi(x)|\, dx (c/\lambda^\nu) \sigma(\delta/8, \beta). \quad \text{(A2.11)}$$

Therefore,

$$C_{\delta,R}(\beta) \leq \frac{1}{\lambda^\nu} \beta e^{2\beta B} \left\{ \int_{|x| > \delta/2} |\phi(x)|\, dx + \int |\phi(x)|\, dx c\sigma(\delta/8, \beta) \right\}. \quad \text{(A2.12)}$$

Upper Bound for $\sum_1^\infty \Delta b_j \frac{\xi^j}{j}$

The same method as above leads immediately to the bound (7.2). From $\sigma(\delta/8, j\beta) \leq 1$, it follows that the last series converges uniformly with respect to r. The right-hand side of (7.2) tends to zero as δ tends to infinity.

Reduced Density Matrices of Quantum Gases. II. Cluster Property

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The reduced density matrices of quantum gases are studied by means of a Wiener integral representation described in a previous paper. They are shown to satisfy a cluster property in the form of an absolute integrability condition of the natural quantum analogues of the Ursell functions, considered as functions of the differences of their arguments. Use is made of the natural transposition to the quantum case of the algebraic formalism introduced by Ruelle in the classical case. By-products are two results on the signs of the coefficients of the Mayer expansion, in the case of Maxwell–Boltzmann and Fermi–Dirac statistics, respectively.

INTRODUCTION

In a previous paper, (Ref. 1, hereafter referred to as I), the reduced density matrices (RDM) for quantum gases have been studied by use of functional integral representation and Banach-space methods. Under suitable restrictions on the interaction, they have been shown to be analytic functions of the activity z in a neighborhood of the origin, and to tend to limits in some sense as the volume becomes infinite. The purpose of the present paper is mainly to prove for these RDM a cluster decomposition property (CP) similar to that obtained by Ruelle (Ref. 2, hereafter referred to as R) for the correlation functions of classical gases. By-products will be bounds on the RDM, more precise than those given in I and two results on the signs of the coefficients of the Mayer expansion of the density (or pressure) as a function of z, valid for purely repulsive interactions, in the case of Maxwell–Boltzmann (MB) and Fermi–Dirac statistics respectively, and similar to that obtained by Groeneveld[3] for classical gases. We shall make use of an algebraic formalism introduced by Ruelle[2,4] for the classical problem, and which can be adapted easily to the quantum-mechanical problem.

As in I, we consider successively MB statistics (Secs. 1–2) and quantum statistics (QS) (Secs. 3–4). The algebraic formalism in the MB case is briefly reviewed in Sec. 1. Easy consequences are the non-integrated form of the Kirkwood–Salzburg (KS) and Mayer–Montroll (MM) equations, as well as the property of the Mayer expansion mentioned above. In Sec. 2, we obtain various bounds for the RDM and we prove the CP. Sections 3 and 4 deal with the QS case and treat the same points in the same order.

It should be noted that the interaction is supposed to satisfy the restrictive conditions of I. In particular, we had to exclude hard cores, as well as attractive interactions in the QS case. It will be shown elsewhere than most of the results of the present paper remain true in these more general situations.

1. ALGEBRAIC PRELIMINARIES IN THE MB CASE

We follow closely R. The notations are those of I when not otherwise stated. The word "measurable" without further specification refers to the conditional Wiener measure $P_{x^m,y^m}(d\omega^m)$ with arbitrary x^m, $y^m \in (R^\nu)^m$ (see I). We note X, Y, $\cdots$, etc. finite sequences of ν-dimensional trajectories. In particular, in Secs. 1–2, X means always $(\omega^m) = (\omega_1, \cdots, \omega_m)$. Let E be the complex vector space of sequences of essentially bounded measurable functionals of m trajectories $h = [h(\omega^m), m = 0, 1, 2, \cdots]$ such that $\int P_{x^m,y^m}(d\omega^m)h(\omega^m)$ be Lebesgue-measurable functions of (x^m, y^m), and E^+ the subspace of those h for which $h_0 = 0$. We define a product in E by $(h_1, h_2) \to h = h_1 * h_2$

$$h(X) = \sum_{Y \subset X} h_1(Y)h_2(X - Y). \tag{1.1}$$

The summation extends over all subsequences Y of X. The trajectories are in the same order in Y and $X - Y$ as they were in X. E then becomes a commutative algebra with unity 1. We define a mapping Γ of E^+ into $1 + E^+$ as the $*$ exponential

$$\Gamma(h) = 1 + h + \frac{h * h}{2!} + \frac{h * h * h}{3!} + \cdots . \tag{1.2}$$

Γ maps E^+ onto $1 + E^+$ and has a unique inverse Γ^{-1}. We now define a linear mapping J of E into the vector space $\bar{E}$ of sequences of Lebesgue measur-

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[1] J. Ginibre, J. Math. Phys. **6**, 238 (1965).
[2] D. Ruelle, Rev. Mod. Phys. **36**, 580 (1964).
[3] J. Groeneveld, Phys. Letters **3**, 50 (1962).
[4] D. Ruelle, Lecture notes of the Theoretical Physics Institute, University of Colorado, Summer 1963.

able functions of m pairs of points (x_j, y_j) in R^ν $(j = 1, \cdots, m; m = 0, 1, 2, \cdots)$ by $h \to \bar{h} = Jh$

$$\begin{cases} \bar{h}_0 = h_0 \\ \bar{h}(x^m, y^m) = \int P_{x^m y^m}(d\omega^m) h(\omega^m) \quad m > 0. \end{cases} \tag{1.3}$$

We define a product $\bar{*}$ in $\bar{E}$ and a mapping $\bar{\Gamma}$ from $\bar{E}^+$ to $\bar{1} + \bar{E}^+$ as the $\bar{*}$ exponential, in the same way as $*$ and Γ were defined, the only difference being the replacement of each trajectory ω_j by a pair of points (x_j, y_j) (which can be thought of as the ends of a trajectory). Then the diagram in Fig. 1 is commutative. The interest of this trivial construction lies in the fact that it has a less trivial analogue in the QS case.

We next define derivations in E as in the classical case[2] by

$$D_\omega h(\omega^m) = h(\omega, \omega_1, \cdots, \omega_m); \tag{1.4}$$

$$D_X h = D_{\omega_1} D_{\omega_2} \cdots D_{\omega_m} h. \tag{1.5}$$

D_ω is linear and satisfies

$$D_\omega(h_1 * h_2) = (D_\omega h_1) * h_2 + h_1 * (D_\omega h_2) \tag{1.6}$$

and

$$D_\omega(\Gamma h) = D_\omega h * \Gamma h \quad \text{for} \quad h \in E^+. \tag{1.7}$$

Now let $\alpha(\omega)$ be a measurable function of one trajectory, such that

$$\int P_{xx}(d\omega)\, dx\, |\alpha(\omega)| < +\infty \tag{1.8}$$

and let α be the sequence of functions $[\alpha(\omega^m), m = 0, 1, 2, \cdots]$ defined by

$$\alpha_0 = 1, \qquad \alpha(\omega^m) = \prod_{i=1}^{m} \alpha(\omega_i). \tag{1.9}$$

To any $h \in E$ we associate the following formal series in z

$$\langle \alpha z, h \rangle = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int P_{x^n, x^n}(d\omega^n)\, dx^n \alpha(\omega^n) h(\omega^n). \tag{1.10}$$

Then

Lemma: $h \to \langle \alpha z, h \rangle$ is a homomorphism of the algebra E into the algebra of formal series in z.

The proof is the same as in R.

Now let $U = (U_m(\omega^m), m = 0, 1, 2, \cdots)$ be a sequence of real measurable functions, satisfying

$$U_0 = 0$$

$$U_m(\omega^m) \geq -m\beta B, \tag{1.11}$$

where B is a constant (real ≥ 0), and let $f \in E$ be

$$\begin{array}{ccc} E^+ & \xrightarrow{\Gamma} & E \\ \Big\downarrow J & & \Big\downarrow J \\ \bar{E}^+ & \xrightarrow{\bar{\Gamma}} & \bar{E} \end{array}$$

FIG. 1

defined by

$$f(\omega^m) = \exp[-U_m(\omega^m)]. \tag{1.12}$$

We are considering here a system of identical particles and $U_m(\omega^m)$ represents the interaction between m particles. Its meaning will become clear later on, when we write its explicit expression under the restriction to two-body forces only, but at the present stage we need only the properties stated above.

Let Λ be a bounded open region (in which the system is supposed to be enclosed) and let $\alpha_\Lambda(\omega)$ be the characteristic function of the set of the continuous trajectories which stay in Λ. Then the grand partition function of the system (GPF) is defined by

$$Z = \langle \alpha_\Lambda z, f \rangle. \tag{1.13}$$

It follows from (1.11) that Z is an entire function of z with $Z(0) = 1$. Its logarithm is therefore holomorphic in a neighborhood of the origin, and

$$Z = \exp \langle \alpha_\Lambda z, g \rangle, \tag{1.14}$$

where

$$g = \Gamma^{-1} f. \tag{1.15}$$

The RDM are defined as the components of $\bar{\rho}_\Lambda = J\rho_\Lambda \in \bar{E}^+$, where $\rho_\Lambda = (\rho_\Lambda(\omega^m), m = 1, 2, \cdots) \in E^+$ is defined by

$$\rho_{\Lambda 0} = 0, \quad \rho_\Lambda(\omega^m) = \alpha_\Lambda(\omega^m) z^m \psi_\Lambda(\omega^m) \quad (m > 0) \tag{1.16}$$

$$\psi_{\Lambda 0} = 1, \quad \psi_\Lambda(X) = \frac{1}{Z} \langle \alpha_\Lambda z, D_X f \rangle \quad (m > 0). \tag{1.17}$$

These definitions are identical with [I: Eqs. (2.8), (2.9)].

We define now $\tilde{\varphi}_X \in E$, χ_Λ, and $\varphi_\Lambda \in E^+$ by

$$\tilde{\varphi}_X = f^{-1} * D_X f, \tag{1.18}$$

$$1 + \rho_\Lambda = \Gamma \chi_\Lambda, \tag{1.19}$$

$$\psi_\Lambda = \Gamma \varphi_\Lambda. \tag{1.20}$$

Then

$$\psi_\Lambda(X) = \langle \alpha_\Lambda z, \tilde{\varphi}_X \rangle, \tag{1.21}$$

$$\chi_\Lambda(X) = \alpha_\Lambda(X) z^m \varphi_\Lambda(X), \tag{1.22}$$

$$\varphi_\Lambda(X) = \langle \alpha_\Lambda z, D_X g \rangle, \tag{1.23}$$

$$\tilde{\varphi}_\omega = D_\omega g. \tag{1.24}$$

The proof is the same as in R.

We define also $\tilde{\chi}_\Lambda = J\chi_\Lambda$, which satisfies

$$\bar{\rho}_\Lambda = \bar{\Gamma}\tilde{\chi}_\Lambda. \tag{1.25}$$

We now restrict ourselves to systems of particles interacting through a two-body potential ϕ satisfying Conditions (a) → (d) of I. Then U becomes

$$U_m(\omega^m) = \sum_{1\le i<j\le m} \int_0^\beta \phi[\omega_i(t) - \omega_j(t)]\, dt. \tag{1.26}$$

From (1.18) and (1.26) one gets easily the non-integrated form of the KS equations

$$\tilde{\varphi}_X(Y) = \exp[-F_1(X)] \times \sum_{S\subset Y} K(\omega_1, S)\tilde{\varphi}_{X'+S}(Y - S), \tag{1.27}$$

where X' is obtained from $X = (\omega^m)$ by removing ω_1.

$X' + S$ is the sequence consisting of the elements of X' and those of S, without changing the order.

$$F_1(X) = \sum_{j=2}^{m} \int_0^\beta \phi[\omega_1(t) - \omega_j(t)]\, dt \tag{1.28}$$

$$K(\omega_1, S) = \prod_{\omega\in S} \left\{\exp\left[-\int_0^\beta \phi[\omega_1(t) - \omega(t)]\, dt\right] - 1\right\} \tag{1.29}$$

The proof is the same as in R.

Similarly, we obtain the nonintegrated form of the Mayer–Montroll equations[5]

$$\tilde{\varphi}_X(Y) = \exp[-U_m(X)] \times \sum_{S\subset Y} K(X, S)\tilde{\varphi}_S(Y - S), \tag{1.30}$$

where

$$K(X, S) = \prod_{\omega\in S} \left(\exp\left\{-\sum_{j=1}^{m} \int_0^\beta \phi[\omega_j(t) - \omega(t)]\, dt\right\} - 1\right). \tag{1.31}$$

We conclude this section with a theorem on the signs of the coefficients of the Mayer expansion for purely repulsive potentials. We first prove

Lemma: Let $Y = \omega^n$ and let $\phi \ge 0$. Then $\tilde{\varphi}_X(Y)$ has the sign of $(-)^n$.

This follows from (1.27) by induction on $m + n$: for $m + n = 1$ either $m = 1$, $n = 0$, $\tilde{\varphi}_1(0) = 1$ or $m = 0$, $n = 1$, $\tilde{\varphi}_0(1) = 0$. $K(\omega_1, S)$ has the sign of $(-)^s$ ($S = \omega^s$) for $\phi \ge 0$, whence the result. We now prove

Theorem: In the expansion of $\rho_\Lambda(\omega^m)$ and $\bar{\rho}_\Lambda(x^m, y^m)$ in power series of z, the coefficient of z^{m+n} has the sign of $(-)^n$. The result holds both for finite and infinite volume. In particular, in the Mayer expansion of the density as a power series of z, the coefficient of z^l has the sign of $(-)^{l+1}$.

This follows immediately from (1.16), (1.17), and (1.21), and the preceding lemma.

[5] J. E. Mayer and E. Montroll, J. Chem. Phys. 9, 2 (1941).

2. BOUNDS ON THE RDM AND CP IN THE MB CASE

The two-body potential ϕ is supposed to satisfy conditions (a) → (d) of I. We first obtain by induction on $m + n$ the following inequality

$$\int |\tilde{\varphi}_X(\omega^n)|\, P_{y^n y^n}(d\omega^n)\, dy^n \le R_{mn}, \tag{2.1}$$

where

$$R_{mn} = n!\, \xi^{m-1} 1/R^{m+n-1} \qquad (m > 1), \tag{2.2}$$

$$R_{1n} = n!\, e^{-2\beta B}\cdot 1/R^n, \tag{2.3}$$

$$R = \xi \exp[-2\beta B - \xi C(\beta)]. \tag{2.4}$$

ξ is real > 0. The best possible value is $\xi = [C(\beta)]^{-1}$.

$$C(\beta) = \frac{1}{\lambda^3}\beta e^{2\beta B}\int |\phi|\, dx$$

appears as an upper bound [I: (A2.6)] for $\sup_{\omega_1} \int P_{yy}(d\omega)\, dy\, |K(\omega_1, \omega)|$ and $\lambda = (\pi\beta)^{\frac{1}{2}}$ is the thermal wavelength. The proof is the same as in R.

A more careful majorization[6] enables us to replace R_{mn} by the better bounds P_{mn}

$$P_{mn} = m(m + n)^{n-1} \times \exp[2(m + n - 1)\beta B][C(\beta)]^n (m > 1), \tag{2.5}$$

$$P_{1n} = (n + 1)^{n-1} \exp[2(n - 1)\beta B][C(\beta)]^n. \tag{2.6}$$

Comparison of (2.1) with (1.16), (1.21) shows that for $|z| < R$ the power series for ψ_Λ and ρ_Λ, as well as the corresponding series for infinite volume, obtained by replacing α_Λ by 1:

$$\psi(X) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int P_{y^n y^n}(d\omega^n)\tilde{\varphi}_X(\omega^n)\, dy^n \tag{2.7}$$

$$\rho_0 = 0 \tag{2.8}$$

$$\rho(X) = z^m \psi(X) \qquad (m > 0) \tag{2.9}$$

are uniformly convergent and bounded by

$$|\psi(X)| \le (\xi^{m-1}/R^{m-1})(1 - |z|/R)^{-1}, \tag{2.10}$$

$$|\rho(X)| \le (|z|/\xi)(|z|/R)^{m-1}\xi^m(1 - |z|/R)^{-1}. \tag{2.11}$$

This bound is better than that given in I (cf. I: 3.19) by a factor $(|z|/R)^{m-1}$. It has been shown in I that when Λ becomes infinite the functions $\rho_\Lambda(\omega^m)$ tend

[6] O. Penrose, J. Math. Phys. 4, 1312 (1963).

to limits uniformly for $|z| \leq R' < R$. Therefore the coefficients

$$\frac{1}{n!}\alpha_\Lambda(X)\int P_{y^n y^n}(d\omega^n)\alpha_\Lambda(\omega^n)\tilde{\varphi}_X(\omega^n)\,dy^n \tag{2.12}$$

tend to the coefficients of the expansion of these limits in powers of z. Therefore these limits coincide with the $\rho(\omega^m)$ defined by (2.9).

In the case of purely repulsive potentials ($\phi \geq 0$) one can get more precise bounds from the MM equations (1.30). We shall obtain by induction on $m + n$:

$$\int |\tilde{\varphi}_X(\omega^n)|\, P_{y^n y^n}(d\omega^n)\,dy^n \leq R'_{mn}\exp\left[-U_m(X)\right] \tag{2.13}$$

Comparing with (1.30) gives the sufficient condition:

$$R'_{mn} \geq \sum_{s=0}^{n} C_n^s R_{s,n-s}[mC(\beta)]^s \tag{2.14}$$

due to

$$\int P_{yy}(d\omega)\,|K(X,\omega)|\,dy \leq mC(\beta). \tag{2.15}$$

(2.14) has the solution, for any $\xi > 0$

$$R'_{mn} = n!\,\xi^{-n}\exp\left[(m+n-1)\xi C(\beta)\right]. \tag{2.16}$$

This is the value taken by R_{mn} for $B = 0$. A more careful majorization[6] enables us to replace R'_{mn} by P'_{mn}

$$P'_{mn} = m(m+n)^{n-1}[C(\beta)]^n. \tag{2.17}$$

For purely repulsive potentials and physical, i.e., real positive values of z, we can obtain better bounds on ρ_Λ directly.[3] From the definitions (1.16), (1.17), and the inequality

$$\exp\left[-U_{m+n}(\omega^{m+n})\right] \leq \exp\left[-U_m(\omega^m)\right]\exp\left[-U_n(\omega^n)\right], \tag{2.18}$$

we obtain immediately

$$\rho_\Lambda(\omega^m) \leq z^m \exp\left[-U_m(\omega^m)\right]. \tag{2.19}$$

From the various bounds on ρ_Λ and the relation $\bar{\rho}_\Lambda = J\rho_\Lambda$, one obtains easily corresponding bounds for the RDM themselves.

We now prove a CP for $\bar{\rho}(x^m, y^m)$, i.e., a property of decrease at infinity of $\bar{\chi}(x^m, y^m)$ defined by $\bar{1} + \bar{\rho} = \bar{\Gamma}\bar{\chi}$. We define χ and φ in the same way as χ_Λ, φ_Λ by

$$1 + \rho = \Gamma\chi, \tag{2.20}$$

$$\chi(X) = z^m\varphi(X), \tag{2.21}$$

$$\varphi(X) = \sum_{n=0}^{\infty}\frac{z^n}{n!}\int P_{y^n y^n}(d\omega^n)D_X g(\omega^n)\,dy^n. \tag{2.22}$$

We first obtain by induction on $m + n$ the following inequality

$$\int |\tilde{\varphi}_X(\omega^n)|\, P_{y^n, y^{n+a^n}}(d\omega^n)\,dy^n \leq R_{mn}\lambda'^n\psi_\beta(a^n), \tag{2.23}$$

where R_{mn} is defined by (2.2), (2.3), and

$$\psi_\beta(a^n) = \prod_{i=1}^{n}\frac{1}{\lambda'}\exp\left[-\frac{a_i^2}{\beta}\right]. \tag{2.24}$$

We have used the following bound, which follows immediately from I: (A2.3)

$$\sup_{\omega_1}\int P_{y,y+a}(d\omega)\,dy\,|K(\omega_1,\omega)| \leq \psi_\beta(a)\beta e^{2\beta B}\int|\phi|\,dx = \lambda'\psi_\beta(a)C(\beta). \tag{2.25}$$

The proof is the same as that of (2.1). From (2.22) we get

$$\int |\varphi(\omega^m)|\, P_{x^{m-1},(x+a)^{m-1}}(d\omega^{m-1})\,dx^{m-1} \leq \sum_{n=0}^{\infty}\frac{|z|^n}{n!}\int P_{x^{m-1},(x+a)^{m-1}}(d\omega^{m-1})\,dx^{m-1} \times P_{y^n y^n}(d\omega^n)\,|D_X g(\omega^n)|. \tag{2.26}$$

Now

$$D_X g(\omega^n) = D_\omega g(\omega^{m-1},\omega^n) = \tilde{\varphi}_\omega(\omega^{m-1},\omega^n). \tag{2.27}$$

Therefore

$$\begin{aligned}\cdots &\leq \sum_{n=0}^{\infty}\frac{|z|^n}{n!}R_{1,m+n-1}\lambda'^{n(m-1)}\psi_\beta(a^{m-1})\\ &\leq \sum_{n=0}^{\infty}\frac{|z|^n}{n!}(m+n-1)!\,e^{-2\beta B}\frac{1}{R^{m+n-1}}\lambda'^{n(m-1)}\psi_\beta(a^{m-1})\\ &\leq (m-1)![e^{-2\beta B}R^{-(m-1)}/(1-|z|/R)^m]\lambda'^{n(m-1)}\psi_\beta(a^{m-1}).\end{aligned} \tag{2.28}$$

Integrating over the last trajectory and comparing with (2.21) we obtain finally

$$\int |\bar{\chi}(x^m, x^m + a^m)|\,dx^{m-1} \leq |z|^m\,(m-1)! \times [e^{-2\beta B}R^{-(m-1)}/(1-|z|/R)^m]\lambda'^{n(m-1)}\psi_\beta(a^m), \tag{2.29}$$

which means that $\bar{\chi}(x^m, y^m)$ is an integrable function of the "distances" between the pairs of variables (x_i, y_i) and has an exponential decrease as a function of the distances of the two points of each pair.

A weaker form of the CP is obtained by integrating over a^m,

$$\int |\bar{\chi}(x^m, y^m)|\,dx^m\,dy^{m-1} \leq |z|^m\,(m-1)! \times [e^{-2\beta B}R^{-(m-1)}/(1-|z|/R)^m]\lambda'^{n(m-1)} \tag{2.30}$$

and will be shown in Sec. 4 to have an analogue in the QS case.

3. ALGEBRAIC PRELIMINARIES IN THE QS CASE

We now develop the corresponding algebra in the QS case. The variables are now trajectories ω of length (defined as the length of the t interval $j\beta$, j integer ≥ 1.) Finite sequences of such trajectories are noted X, Y, $\cdots$, etc., or (ω^m, j^m), by which is meant that the trajectory ω_i has the length $j_i\beta$ $(i = 1, \cdots, m)$.

Let A_0 be the complex vector space of sequences of essentially bounded measurable functionals of m trajectories $h = [h(\omega^m, j^m), j_i = 1, 2, \cdots; m = 0, 1, \cdots]$ such that $\int P^{j^m}_{x^m, y^m}(d\omega^m)\, h(\omega^m, j^m)$ be Lebesgue measurable functions of (x^m, y^m). For $m = 0$, there is only one component, which is a complex number h_0. Let A_0^+ be the subspace of these h for which $h_0 = 0$. We define a product $*$ in A_0 by $(h_1, h_2) \to h = h_1 * h_2$

$$h(X) = \sum_{Y \subset X} h_1(Y) h_2(X - Y). \tag{3.1}$$

E then becomes a commutative algebra with unity 1. We define a mapping Γ as the $*$ exponential. Γ maps A_0^+ onto $1 + A_0^+$ and has a unique inverse Γ^{-1}.

The subset of those $h \in A_0$ the components of which are totally symmetric with respect to their arguments is a subalgebra $A \subset A_0$. From now on, we consider only A.

The order of the trajectories in the sequences X being now immaterial, the variables j^m can be described by a partition of m into integers γ_i such that $\sum \gamma_i = m$, j entering γ_j times in j^m. These $\gamma = (\gamma_i)$ can be conveniently thought of as classes of permutations of $|\gamma| = \sum j\gamma_i$ variables consisting of γ_j cycles of j elements $(j = 1, 2, \cdots)$ (see I—Sec. 5). From now on, we use systematically the following notations:

$$X = \omega^\gamma = (\omega^m, j^m) \quad \Sigma\gamma_i = m, \quad |\gamma| = \Sigma j\gamma_i = q.$$

$$Y = \omega^\delta = (\omega^n, j^n) \quad \Sigma\delta_i = n, \quad |\delta| = \Sigma j\delta_i = r.$$

$\gamma = \gamma' + \gamma''$ means: $\gamma_i = \gamma_i' + \gamma_i''$ for all j.

$\gamma' \leq \gamma$ means: $\gamma_i' \leq \gamma_i$ for all j.

If $\gamma' \leq \gamma$, $\gamma - \gamma'$ is the partition γ'' defined by $\gamma_i'' = \gamma_i - \gamma_i'$ for all j. Now let $\bar{E}$ be the complex vector space of sequences of Lebesgue measurable functions of m pairs of points $(x_j, y_j) \in R^\nu$, $j = 1, \cdots, m$; $m = 0, 1, \cdots$, which are totally ϵ-symmetric (symmetric for $\epsilon = +1$, antisymmetric for $\epsilon = -1$) with respect to the variables x and y separately. It is natural[7] to define a product in $\bar{E}$ by

$$\bar{h}_1, \bar{h}_2 \to \bar{h} = \bar{h}_1 \bar{*} \bar{h}_2$$
$$\bar{h}(\bar{X}) = \sum_{\bar{S}} \epsilon^{\bar{S}} h_1(\bar{S}) h_2(\bar{X} - \bar{S}), \tag{3.2}$$

where $\bar{X} = (x^m, y^m)$.

$\bar{S} = (x^s, y^s)$ is obtained by selecting independently s variables x out of m, and s variables y out of m, $\bar{X} - \bar{S}$ consists of the remaining variables. The variables x and y are in the same order in $\bar{S}$ and in $\bar{X} - \bar{S}$ as they were in $\bar{X}$.

$\epsilon^{\bar{S}}$ is $+1$ for $\epsilon = +1$, and the signature of the product of the permutations which transform x^m into x^s, x^{m-s} and y^m into y^s, y^{m-s} respectively, for $\epsilon = -1$. $\bar{E}$ is then a commutative algebra with unity $\bar{1}$. Let $\bar{E}^+$ be the subspace of those $\bar{h} \in \bar{E}$ for which $\bar{h}_0 = 0$. We define the mapping $\bar{\Gamma}$ from $\bar{E}^+$ to $\bar{1} + \bar{E}^+$ as the $\bar{*}$ exponential. One has for instance, for $\bar{h} \in \bar{E}^+$

$$(\bar{\Gamma}\bar{h})_0 = 1,$$
$$(\bar{\Gamma}\bar{h})(x, y) = \bar{h}(x, y),$$
$$(\bar{\Gamma}\bar{h})(x_1y_1, x_2y_2) = \bar{h}(x_1y_1, x_2y_2) + \bar{h}(x_1, y_1)\bar{h}(x_2, y_2) + \epsilon\bar{h}(x_1y_2)\bar{h}(x_2, y_1). \tag{3.3}$$

$\bar{\Gamma}$ is one to one from $\bar{E}^+$ onto $\bar{1} + \bar{E}^+$ and has a unique inverse $\bar{\Gamma}^{-1}$.

We next define a linear mapping J from A to $\bar{E}$: $h \in A \to \bar{h} = Jh \in \bar{E}$ by

$$\begin{cases} \bar{h}_0 = h_0 \\ \bar{h}(x^m, y^m) = [\sum_\pi (\epsilon)^\pi]_m \\ \qquad \times \sum_{j^m} \epsilon^{q+m} \int P^{j^m}_{x^m, \pi(y^m)}(d\omega^m) h(\omega^m, j^m). \end{cases} \tag{3.4}$$

The first sum extends over all permutations π of m variables. The unexplained notations are the same as in I [see I: (5.4)]. J is not defined on the whole of A. However, it is easy to exhibit a family of subalgebras of A where J is defined. For any real ξ $(0 < \xi < 1)$ and for any sequence $(\sigma) = (\sigma_0, \sigma_1, \cdots)$ of strictly positive real numbers, we define $E_{(\sigma)\xi}$ as the linear space of those $h \in A$ for which

$$||h||_{(\sigma)\xi} = \sup_{\omega^\gamma} \frac{1}{\sigma_m \xi^q} \operatorname{ess\,sup} |h(\omega^\gamma)| < +\infty. \tag{3.5}$$

$E_{(\sigma)\xi}$ is a Banach space with $||h||_{(\sigma)\xi}$ taken as the norm of h. J is defined in each $E_{(\sigma)\xi}$ and for $h \in E_{(\sigma)\xi}$, we have

$$|Jh(x^m, y^m)| \leq \sigma_m m!\, ||h||_{(\sigma)\xi} \{\sum_1^\infty \xi^j / j^{\nu/2}\}^m \lambda^{-\nu m}. \tag{3.6}$$

(One could define Banach spaces $\bar{E}_{(\sigma)\xi} \subset \bar{E}$ such that J be a continuous mapping from $E_{(\sigma)\xi}$ to $\bar{E}_{(\sigma)\xi}$, but we do not make use of this fact.)

[7] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959). S. Weinberg, Phys. Rev. **133**, B232 (1964).

We next define $\mathcal{E}_\xi = \bigcup_{(\sigma)} E_{(\sigma)\xi}$. $\mathcal{E}_\xi$ is a vector space. (The most natural topology for $\mathcal{E}_\xi$ is the inductive limit of the topologies of the $E_{(\sigma)\xi}$; $\mathcal{E}_\xi$ is then a locally convex vector space.[8] We do not make use of this fact.) As an immediate consequence of the following lemma, $\mathcal{E}_\xi$ is a subalgebra of A.

Lemma: If $h' \in E_{(\sigma')\xi}$, $h'' \in E_{(\sigma'')\xi}$, then $h = h' * h'' \in E_{(\sigma)\xi}$, where (σ) is defined by

$$\sigma_m = \sum_{m'=0}^{m} C_m^{m'} \sigma'_{m'} \sigma''_{m-m'} \tag{3.7}$$

and $||h||_{(\sigma)\xi} \leq ||h'||_{(\sigma')\xi} ||h''||_{(\sigma'')\xi}$.

In fact, let $|h'(X)| \leq ||h'||_{(\sigma')\xi} \sigma'_m \xi^q$

$$|h''(X)| \leq ||h''||_{(\sigma'')\xi} \sigma''_m \xi^q.$$

Then

$$\begin{aligned} |h(X)| &\leq \sum_{S \subset X} |h'(S)|\, |h''(X - S)| \\ &= \sum_{\omega^{\gamma'} \subset \omega^{\gamma}} |h'(\omega^{\gamma'})|\, |h''(\omega^{\gamma - \gamma'})| \\ &\leq ||h'||_{(\sigma')\xi}\, ||h''||_{(\sigma'')\xi} \xi^q \\ &\quad \times \sum_{\gamma' \leq \gamma} \prod_j C_{\gamma_j}^{\gamma'_j} \sigma'_{m'} \sigma''_{m-m'}, \end{aligned} \tag{3.8}$$

where $m' = \sum \gamma'_j$. The last sum in (3.8) can be written as:

$$\sum_{m'=0}^{m} \sigma'_{m'} \sigma''_{m-m'} \text{ coef. of } z^{m'} \text{ in } \sum_{\gamma' \leq \gamma} \prod_j (C_{\gamma_j}^{\gamma'_j} z^{\gamma'_j}). \tag{3.9}$$

The last sum in (3.9) factorizes into the product of the contributions of the various j, each of which is equal to $(1 + z)^{\gamma'_j}$, and is therefore equal to $(1 + z)^{m'}$. From this the lemma follows immediately.

J is then defined on each algebra $\mathcal{E}_\xi$, and therefore also on the algebra $\mathcal{E} = \bigcup_{0<\xi<1} \mathcal{E}_\xi$. We next show that Γ maps each $\mathcal{E}_\xi^+$ into $1 + \mathcal{E}_\xi^+$. In fact, let $h \in E_{(\sigma)\xi}^+$:

$$\begin{cases} |h(X)| \leq L \sigma_m \xi^q & \text{where } L = ||h||_{(\sigma)\xi} \\ h_0 = 0. \end{cases}$$

Repeated use of the preceding lemma gives

$$|h^{*k}(X)| \leq L^k \xi^q \sum_{(m_r)} \sigma_{m_1} \cdots \sigma_{m_k} \frac{m!}{m_1! \cdots m_k!} \tag{3.10}$$

where the last sum extends over the partitions (m_r) of m ($m = m_1 + \cdots + m_k$) such that $m_r \geq 1$ for $r = 1, \cdots, k$. The last restriction comes from $h_0 = 0$ and implies in particular that the right-hand side of (3.10) is zero unless $k \leq m$. Then

$$\begin{aligned} &|\Gamma h(X)| \\ &\leq \xi^q \sum_{k=0}^{\infty} \frac{L^k}{k!} \sum_{(m_r)} \sigma_{m_1} \cdots \sigma_{m_k} \frac{m!}{m_1! \cdots m_k!}. \end{aligned} \tag{3.11}$$

Due to the condition $k \leq m$, the series in (3.11) is in fact a finite sum. For fixed h, therefore for fixed L and (σ), it depends only on m. Therefore $\Gamma h \in E_{(\sigma')\xi}$ for some (σ') and therefore $\Gamma h \in \mathcal{E}_\xi$. Consequently, $J\Gamma$ is defined on each $\mathcal{E}_\xi^+$ and therefore also on $\mathcal{E}^+$. The interest of the preceding considerations comes from the

Theorem: J is a homomorphism of the algebra $\mathcal{E}$ into the algebra $\bar{E}$.

Proof: The only nontrivial point is to show that for $h_1, h_2 \in \mathcal{E}$,

$$J(h_1 * h_2) = (Jh_1) \bar{*} (Jh_2). \tag{3.12}$$

In fact, let $\bar{X} = (x^m, y^m)$.

$$\begin{aligned} J(h_1 * h_2)(\bar{X}) &= (\sum_{\pi} \epsilon^{\pi})_m \sum_{j^m} \epsilon^{q+m} \\ &\quad \times \int P^{j^m}_{x^m, \pi(y^m)}(d\omega^m) \sum_{S \subset X} h_1(S) h_2(X - S). \end{aligned} \tag{3.13}$$

We can use the same labeling for x^m and ω^m. Choosing $S \subset X$ is then equivalent to the choice of a subfamily $x^s \subset x^m$ which will be the x part of an $\bar{S}$. The sum over j^m is irrelevant in the present proof. Now for a given choice of x^s, any permutation π_m of the y's is expressible in a unique way as a product $\pi_m = \pi_s \pi_{m-s} \pi'$, where π_s and π_{m-s} act only on the subfamilies y^s and y^{m+s} of y^m which will be matched to x^s and x^{m-s} respectively, and where π' does not change the relative order of the y's in each of these two subfamilies.

The summations on π_s and π_{m-s} for fixed π', together with the sum over j^m and the integration, when applied to $h_1(S)$ and $h_2(X - S)$, give $Jh_1(\bar{S})$ and $Jh_2(\bar{X} - \bar{S})$ respectively. On the other hand, the summation over S and over π', in view of $\epsilon^{\pi'} = \epsilon^{\bar{S}}$, give the definition of the $\bar{*}$ product; whence the result.

From the preceding theorem it follows that $J\Gamma = \bar{\Gamma} J$ wherever both sides are defined, and in particular in $\mathcal{E}^+$. Therefore the diagram of Fig. 2 is commutative.

We next define derivations in A as previously.

$$D_{(\omega, k)} h(\omega^m, j^m) = h(\omega, k; \omega^m j^m) \tag{3.14}$$

$$D_X h = D_{(\omega_1, j_1)} \cdots D_{(\omega_m, j_m)} h. \tag{3.15}$$

[8] Bourbaki, *Espaces vectoriels topologiques*, (Hermann & Cie., Paris, 1953).

$$\begin{array}{ccc} \mathcal{E}^+ & \xrightarrow{\Gamma} & \mathcal{E} \\ \Big\downarrow J & & \Big\downarrow J \\ \bar{E}^+ & \xrightarrow{\Gamma} & \bar{E} \end{array}$$

Fig. 2

The functions in A are symmetric, therefore the derivations commute. As previously

$$D_{(\omega,k)}(h_1 * h_2) = (D_{(\omega,k)}h_1) * h_2 + h_1 * D_{(\omega,k)}h_2 \tag{3.16}$$

$$D_{(\omega,k)}(\Gamma h) = D_{(\omega,k)}h * \Gamma h \quad \text{for} \quad h \in A^+. \tag{3.17}$$

Now let $[\alpha_j(\omega),\ j = 1, 2, \cdots]$ be a sequence of measurable functions of one trajectory ω of length $j\beta$ such that

$$\int P^j_{xx}(d\omega)\, dx\, |\alpha_j(\omega)| < +\infty \tag{3.18}$$

and let α be the sequence of functions $[\alpha(\omega^m, j^m),\ m = 0, 1, \cdots]$ defined by

$$\alpha_0 = 1 \qquad \alpha(\omega^m, j^m) = \prod_{k=1}^{m} \alpha_{j_k}(\omega_k). \tag{3.19}$$

To any $h \in A$ we associate the following formal series in z

$$\langle \alpha z, h\rangle_\epsilon = \sum_{r=0}^{\infty} z^r \sum_{\delta(r)} \prod_j \frac{1}{\delta_j!} \times \int \left(\frac{\epsilon^{j+1}}{j} P^j_{xx}(d\omega)\, dx \alpha_j(\omega)\right)^{\delta_j} h(\omega^\delta) \tag{3.20}$$

or

$$\langle \alpha z, h\rangle_\epsilon = \sum_{r=0}^{\infty} z^r \sum_{\delta(r)} \int d_\epsilon\omega^\delta \alpha(\omega^\delta) h(\omega^\delta),$$

where $\sum_{a(b)}$ means sum over a, b being held fixed; $\epsilon = \pm 1$ and

$$d_\epsilon\omega^\delta = \prod_j (1/\delta_j!)[(\epsilon^{j+1}/j)P^j_{xx}(d\omega)\, dx]^{\delta_j}. \tag{3.21}$$

Then we have

Lemma: $h \to \langle \alpha z, h\rangle_\epsilon$ is a homomorphism of the algebra A into the algebra of formal series in z.

Proof: The only nontrivial point is to show that for $h_1, h_2 \in A$,

$$\langle \alpha z, h_1 * h_2\rangle_\epsilon = \langle \alpha z, h_1\rangle_\epsilon \langle \alpha z, h_2\rangle_\epsilon \tag{3.22}$$

Now:

$$\langle \alpha z, h_1 * h_2\rangle_\epsilon = \sum_{r=0} z^r \sum_{\delta(r)} \int d_\epsilon\omega^\delta \alpha(\omega^\delta) \times \sum_{\omega^{\delta'} \subset \omega^\delta} h_1(\omega^{\delta'}) h_2(\omega^{\delta-\delta'}) = \sum_{r=0}^{\infty} z^r \sum_{\delta(r)} \int d_\epsilon\omega^\delta \sum_{\delta' \le \delta} \alpha(\omega^{\delta'})\alpha(\omega^{\delta-\delta'}) \prod_j C^{\delta'_j}_{\delta_j} h_1(\omega^{\delta'}) h_2(\omega^{\delta-\delta'}).$$

Now

$$\prod_j C^{\delta'_j}_{\delta_j} d_\epsilon\omega^\delta = d_\epsilon\omega^{\delta'} d_\epsilon\omega^{\delta-\delta'}, \tag{3.23}$$

whence the result.

Now let $U = (U(\omega^\nu))$ be a sequence of real measurable functions satisfying

$$U_0 = 0, \qquad U(\omega^\nu) \ge -q\beta B, \tag{3.24}$$

where B is a constant (real ≥ 0) and let $f \in A$ be defined by

$$f(\omega^\nu) = \exp[-U(\omega^\nu)]. \tag{3.25}$$

As previously, U represents the interactions of a system of identical particles (bosons for $\epsilon = +1$, fermions for $\epsilon = -1$), and will be given an explicit expression later on for a system with two-body forces only.

Let Λ be a bounded open region and $\alpha_j(\omega)$ be the characteristic function of the set of the continuous trajectories of length $j\beta$ which stay in Λ. The grand partition function (GPF) of the system is defined by

$$Z_\epsilon = \langle \alpha_\Lambda z, f\rangle_\epsilon. \tag{3.26}$$

It follows from (3.24) that Z_ϵ is an analytic function of z for $|z| < e^{-\beta B}$ and satisfies I: (5.12)

$$|Z_\epsilon| \le \exp\left\{\frac{V}{\lambda^\nu} \sum_{j=1} \frac{(|z|\, e^{\beta B})^j}{j^{\nu/2+1}}\right\} \tag{3.27}$$

and $Z_\epsilon(0) = 1$. (Here V is the volume of Λ.) Therefore $\log Z_\epsilon$ is analytic in a neighborhood of the origin and

$$Z_\epsilon = \exp\langle \alpha_\Lambda z, g\rangle_\epsilon, \quad \text{where} \quad g = \Gamma^{-1} f. \tag{3.28}$$

The RDM are now defined as the components of $\bar{\rho}_\Lambda = J\rho_\Lambda$ in terms of the correlation functionals $(\rho_\Lambda(\omega^m, j^m),\ m = 1, \cdots) = \rho_\Lambda \in A^+$, where

$$\rho_{\Lambda 0} = 0, \quad \rho_\Lambda(X) = \alpha_\Lambda(X) z \psi_\Lambda(X) \quad (m > 0) \tag{3.29}$$

$$\psi_{\Lambda 0} = 1, \quad \psi_\Lambda(X) = (1/Z_\epsilon)\langle \alpha_\Lambda z, D_X f\rangle_\epsilon \quad (m > 0). \tag{3.30}$$

We define as previously $\tilde{\varphi}_X \in A$, χ_Λ and $\varphi_\Lambda \in A^+$, by

$$\tilde{\varphi}_X = f^{-1} * D_X f \tag{3.31}$$

$$1 + \rho_\Lambda = \Gamma\chi_\Lambda \tag{3.32}$$

$$\psi_\Lambda = \Gamma\varphi_\Lambda. \tag{3.33}$$

Then

$$\psi_\Lambda(X) = \langle \alpha_\Lambda z, \tilde{\varphi}_X \rangle_\epsilon \tag{3.34}$$

$$\chi_\Lambda(X) = \alpha_\Lambda(X) z^q \varphi_\Lambda(X) \tag{3.35}$$

$$\varphi_\Lambda(X) = \langle \alpha_\Lambda z, D_X g \rangle_\epsilon . \tag{3.36}$$

We now restrict ourselves to systems of particles interacting through a two-body potential ϕ satisfying Conditions (a) $\rightarrow$ (d) of I. U becomes:

$$U(X) = \int_0^\beta dt \Big\{ \sum_{k=1}^{m} \sum_{0 \le i < i' \le i_{k-1}} \phi[\omega_k(t + j\beta) - \omega_k(t + j'\beta)] + \sum_{1 \le k < k' \le m} \sum_{i=0}^{i_k - 1} \sum_{i'=0}^{i_{k'}-1} \phi[\omega_k(t + j\beta) - \omega_{k'}(t + j'\beta)] \Big\}. \tag{3.37}$$

From (3.31), one gets the nonintegrated form of the KS equations [I: (6.8)]

$$\tilde{\varphi}_X(Y) = \exp[-F_1(X)] \times \sum_{S \subset Y} K(\omega_1, j_1, S) \tilde{\varphi}_{X'+S}(Y - S), \tag{3.38}$$

with

$$F_1(X) = \int_0^\beta dt \Big\{ \sum_{0 \le i < i' \le i_1 - 1} \phi[\omega_1(t + j\beta) - \omega_1(t + j'\beta)] + \sum_{k=2}^{m} \sum_{i=0}^{i_1 - 1} \sum_{i'=0}^{i_k - 1} \phi[\omega_1(t + j\beta) - \omega_k(t + j'\beta)] \Big\} \tag{3.39}$$

$$K(\omega_1, j_1, S) = \prod_{\omega, i \in S} \Big\{ \exp\Big[-\int_0^\beta dt \times \sum_{l=0}^{i_1 - 1} \sum_{l'=0}^{j-1} \phi[\omega_1(t + l\beta) - \omega(t + l'\beta)] \Big] - 1 \Big\} \tag{3.40}$$

The proof is the same as previously.

Similarly, we obtain the Mayer–Montroll equations in nonintegrated form:

$$\tilde{\varphi}_X(Y) = \exp[-U(X)] \times \sum_{S \subset Y} \tilde{\varphi}_S(X - S) K(X, S), \tag{3.41}$$

where

$$K(X, S) = \prod_{(\omega, i) \in S} \Big\{ \exp\Big[-\int_0^\beta dt \times \sum_{k=1}^{m} \sum_{l=0}^{i_k - 1} \sum_{l'=0}^{j-1} \phi[\omega_k(t + l\beta) - \omega(t + l'\beta)] \Big] - 1 \Big\}. \tag{3.42}$$

We conclude this section with an algebraic result valid for purely repulsive potentials only. We first prove:

Lemma: Let $\phi \ge 0$. Then the sign of $\tilde{\varphi}_X(Y)$ is $(-)^n$. [Recall that $Y = (\omega^n, j^n)$.] $K(\omega_1 j_1, S)$ has the sign of $(-)^s$ and the result follows by induction on $m + n$ as previously.

Then we have:

Lemma: Let $\phi \ge 0$. In the expansion of $\rho_\Lambda(\omega^\gamma)$ in powers of z, for fermions only ($\epsilon = -1$), the coefficient of z^{q+r} has the sign of $(-)^r$.

We get from (3.34)

$$\psi(X) = 1 + \sum_{r=1}^{\infty} z^r \sum_{\delta(r)} \int d_\epsilon \omega^\delta \alpha_\Lambda(\omega^\delta) \tilde{\varphi}_X(\omega^\delta). \tag{3.43}$$

Now $d_\epsilon \omega^\delta$ contains $\epsilon^{\sum (i+1)\delta_i} = \epsilon^{r+n}$.

$\tilde{\varphi}_X(\omega^\delta)$ has the sign of $(-)^n$. Therefore for bosons ($\epsilon = +1$) we can conclude nothing. For fermions, all terms with given r have the same sign, and the coefficient of z^r has the sign $(-)^r$, whence the result.

Theorem: In the Mayer expansion $\bar{\rho}_\Lambda(x, x) = \sum_l b_l z^l$, for fermions with repulsive interactions ($\phi \ge 0$), b_l has the sign of $(-)^{l+1}$; $|b_l| \ge |b_l^{(0)}|$, where $b_l^{(0)}$ is the corresponding coefficient for a free gas at the same temperature.

This follows immediately from the preceding lemma, applied to

$$\rho_\Lambda(\omega, j) = \alpha_\Lambda(\omega) z^j \Big[1 + \sum_{1}^{\infty} (-)^r z^r \times \text{positive coefficient} \Big] \tag{3.44}$$

$$\bar{\rho}_\Lambda(x, y) = \sum_{j=1}^{\infty} (-)^{j+1} \int P_{xy}^j(d\omega) \rho_\Lambda(\omega, j). \tag{3.45}$$

All the terms contributing to a given power of z have the same sign, and the first term in the expansion (3.44) gives the free-gas part.

4. BOUNDS ON THE RDM AND CP IN THE QS CASE

Throughout this section, the potential ϕ satisfies Conditions (a) $\rightarrow$ (d') of I. In particular, ϕ is repulsive ($\phi \ge 0$). The notations are these of Sec. 3. We now deduce bounds for ρ_Λ from the KS equations (3.38). We first look for bounds of the type

$$\int |\tilde{\varphi}_X(\omega^\delta)| \, d_+\omega^\delta \le P(\gamma, \delta). \tag{4.1}$$

We proceed by induction on $q + r$. A sufficient condition follows from (3.38):

$$P(\gamma, \delta) \ge \exp[-F_1(X)] \sum_{\delta' \le \delta} P(\gamma' + \delta', \delta - \delta') \times \int d_+\omega^{\delta'} \, |K(\omega_1, k; \omega^{\delta'})|, \tag{4.2}$$

where $\omega^{\gamma'}$ is obtained from ω^{γ} by removing (ω_1, k). (4.2) and the inequality I (A2.8)

$$\frac{1}{j}\int P^j_{xx}(d\omega)\,dx\,|K(\omega_1, k; \omega, j)| \leq k\,\frac{C(\beta)}{j^{\nu/2}}, \tag{4.3}$$

where

$$C(\beta) = (1/\lambda^{\nu})\beta\int |\phi(x)|\,dx, \tag{4.4}$$

give the sufficient condition:

$$P(\gamma, \delta) \geq \sup_{k(\gamma_k \geq 1)} \sum_{\delta' \leq \delta} P(\gamma' + \delta', \delta - \delta') \times \prod_j (1/\delta'_j!)[kC(\beta)/j^{\nu/2}]^{\delta'_j}. \tag{4.5}$$

Instead of solving for the uninteresting $P(\gamma, \delta)$, we next look for bounds of the type

$$\sup_{\gamma(q)} \sum_{\delta(r)} P(\gamma, \delta) \leq P(q, r). \tag{4.6}$$

Comparison with (4.5) gives the sufficient condition

$$P(q, r) \geq \sup_{1\leq k\leq q} \sum_{r'=0}^{r} P(q - k + r', r - r') \times \sum_{\delta'(r')} \prod_j \frac{1}{\delta'_j!}\left[k\,\frac{C(\beta)}{j^{\nu/2}}\right]^{\delta'_j}, \tag{4.7}$$

or equivalently

$$P(q, r) \geq \sup_{1\leq k\leq q} \sum_{r'=0}^{r} P(q - k + r', r - r') \times \text{coefficient of } \xi^{r'} \text{ in the expansion of } \exp(Dk) \text{ as a power series in } \xi, \tag{4.8}$$

where

$$D = D(\beta, \xi) = C(\beta)\sum_{j=1} \xi^j/j^{\nu/2}. \tag{4.9}$$

This series converges for $|\xi| \leq 1$. (4.8) suggests the obvious solution

$$P(q, r) = \text{const} \times e^{(q+r)D}/\xi^r. \tag{4.10}$$

The induction procedure begins at $q + r = 1$, which implies $q = 1$, $r = 0$, $P(1, 0) = 1$. Therefore we can take the constant as $\exp(-D)$. Finally

$$\sup_{\omega^{\gamma}(q)} \sum_{\delta(r)} \int d_+\omega^{\delta}\,|\tilde{\varphi}_X(\omega^{\delta})| \leq \frac{\exp[(q + r - 1)D]}{\xi^r}. \tag{4.11}$$

Comparison of (4.11) with (3.29), (3.34) shows that for $|z| < R = \xi \exp(-D)$, the power series for ψ_Λ and ρ_Λ, as well as the corresponding series for infinite volume obtained by replacing α_Λ by 1:

$$\psi(X) = \sum_0^{\infty} z^r \sum_{\delta(r)} \int d_+\omega^{\delta}\tilde{\varphi}_X(\omega^{\delta}) \tag{4.12}$$

$$\rho(X) = z^q\psi(X) \tag{4.13}$$

converge uniformly and satisfy

$$|\psi(X)| \leq (\xi/R)^{q-1}(1 - |z|/R)^{-1}; \tag{4.14}$$

$$|\rho(X)| \leq (|z|/\xi)\xi^q(|z|/R)^{q-1}(1 - |z|/R). \tag{4.15}$$

The last bound is better than that given in I by a factor $(|z|/R)^{q-1}$. The ρ defined by (4.15) coincide with the limits of ρ_Λ obtained in I as the volume becomes infinite. The proof is the same as previously.

We can obtain better bounds from the Mayer–Montroll equations (3.41). (The potential ϕ is repulsive, $\phi \geq 0$.) Similar methods show that

$$\sup_{\omega^{\gamma}(q)} \sum_{\delta(r)} \int d_+\omega^{\delta}\,|\tilde{\varphi}_X(\omega^{\delta})| \leq \frac{\exp[(q + r - 1)D]}{\xi^r}\exp[-U(X)] \tag{4.16}$$

$$|\rho(X)| \leq (|z|/\xi)\xi^q(|z|/R)^{q-1}1/(1 - |z|/R) \times \exp[-U(X)]. \tag{4.17}$$

For physical, i.e., real positive values of z, in the case of Bose statistics only, we can obtain better bounds on ρ_Λ directly.[3] From the definitions (3.29), (3.30), and the inequality

$$\exp[-U(\omega^{\gamma+\delta})] \leq \exp[-U(\omega^{\gamma})]\exp[-U(\omega^{\delta})], \tag{4.18}$$

we obtain immediately

$$\rho_\Lambda(\omega^{\gamma}) \leq z^q \exp[-U(\omega^{\gamma})]. \tag{4.19}$$

From the various bounds on ρ_Λ and the relation $\bar{\rho}_\Lambda = J\rho_\Lambda$, one obtains as previously corresponding bounds for the RDM themselves.

We now prove a CP for $\bar{\rho}(x^m, y^m)$, i.e., a property of decrease at infinity of the components $\bar{\chi}(x^m, y^m)$ of $\bar{\chi} \in \bar{E}^+$ defined by

$$\bar{1} + \bar{\rho} = \bar{\Gamma}\bar{\chi}. \tag{4.20}$$

We define χ and φ in the same way as χ_Λ and φ_Λ, by

$$1 + \rho = \Gamma\chi \tag{4.21}$$

$$\chi(X) = z^q\varphi(X) \tag{4.22}$$

$$\varphi(X) = \sum_{r=0}^{\infty} z^r \sum_{\delta(r)} \int d_c\omega^{\delta} D_X g(\omega^{\delta}). \tag{4.23}$$

More precisely, we prove that $\bar{\chi}(x^m, y^m)$ is an integrable function of the differences of its arguments by obtaining a finite upper bound for the integral

$$J_m = \int dx^m\,dy^{m-1}\,|\bar{\chi}(x^m, y^m)|. \tag{4.24}$$

Let

$$d\omega^\delta = \prod_i \frac{1}{\delta_i!} [P^i_{xy}(d\omega)\, dx\, dy]^{\delta_i} \tag{4.25}$$

and

$$T = \omega^\theta \quad \theta = (\theta_i) \quad |\theta| = \sum j\theta_i = s.$$

We first prove the following

Lemma:

$$\sum_{q+r=p} \sup_{T(s)} \sum_{\gamma(m,q)} \sum_{\delta(r)} \int d\omega^\gamma\, d_+\omega^\delta\, |\tilde\varphi_T(X, Y)|$$

$$\leq \exp[(p+s-1)D] \frac{1}{\xi^p} \frac{1}{m!} \left[(p+s)A \frac{\xi}{(1-\xi)^2}\right]^m, \tag{4.26}$$

where

$$A = \lambda' C(\beta) = \beta \int |\phi|\, dx. \tag{4.27}$$

Proof: We first look for bounds of the type

$$\int d\omega^\gamma\, d_+\omega^\delta\, |\tilde\varphi_T(X, Y)| \leq P(\theta, \gamma, \delta). \tag{4.28}$$

We proceed by induction on $s + q + r$. We rewrite the KS equations as

$$\tilde\varphi_T(X, Y) = \exp[-F_1(T)] \sum_{\substack{X'\subset X \\ Y'\subset Y}} K(\omega_1, k, X')$$

$$\times K(\omega_1, k, Y')\tilde\varphi_{T'+X'+Y'}(X - X', Y - Y'), \tag{4.29}$$

where $X' = \omega^{\gamma'}$, $Y' = \omega^{\delta'}$, and T' is obtained from T by removing (ω_1, k). (4.28) and (4.29) give the sufficient condition on P:

$$P(\theta, \gamma, \delta)$$

$$\geq \sup_{k(\theta_k\geq 1)} \sum_{\gamma'\leq\gamma} \sum_{\delta'\leq\delta} P(\theta' + \gamma' + \delta', \gamma - \gamma', \delta - \delta')$$

$$\times \int d\omega^{\gamma'}\, |K(\omega_1, k, \omega^{\gamma'})| \int d_+\omega^{\delta'}\, |K(\omega_1, k, \omega^{\delta'})|. \tag{4.30}$$

From (4.3) and the similar inequality:

$$\int P^i_{xy}(d\omega)\, dx\, dy\, |K(\omega_1, k, \omega, j)| \leq kjA, \tag{4.31}$$

where A is defined by (4.27), and which is easily obtained by the method of I (Appendix 2), we obtain the sufficient condition

$$P(\theta, \gamma, \delta) \geq \sup_{k(\theta_k\geq 1)} \sum_{\gamma'\leq\gamma} \sum_{\delta'\leq\delta}$$

$$P(\theta' + \gamma' + \delta', \gamma - \gamma', \delta - \delta')(kA)^{m'}$$

$$\times \prod_i \frac{1}{\gamma_i'!} j^{\gamma_i'} \prod_i \frac{1}{\delta_i'!} \left[kC(\beta) \frac{1}{j^{p/2}}\right]^{\delta_i'}. \tag{4.32}$$

The next step is to look for bounds of the type

$$\sup_{\theta(s)} \sum_{\gamma(m,q)} \sum_{\delta(r)} P(\theta, \gamma, \delta) \leq P(s, q, m, r). \tag{4.33}$$

From (4.32) we get by summation over γ, δ, the sufficient condition

$$P(s, q, m, r) \geq \sup_{1\leq k\leq s} \sum_{r'=0}^{r} \sum_{m'=0}^{m} \sum_{q'=m'}^{q}$$

$$P(s - k + q' + r', q - q', m - m', r - r')$$

$$\times \text{coef. of } \xi^{r'} \text{ in } \exp(kD) \times \frac{(kA)^{m'}}{m'!}$$

$$\times \text{coef. of } \xi^{q'} \text{ in } \left(\sum_1^\infty j\xi^j\right)^{m'}. \tag{4.34}$$

The last step is to look for bounds of the type

$$\sum_{q\geq m,\ r\geq 0,\ q+r=p} P(s, q, m, r) \leq P(s, m, p). \tag{4.35}$$

From (4.34) we get the sufficient condition

$$P(s, m, p) \geq \sup_{1\leq k\leq s} \sum_{m'=0}^{m} \sum_{p'=m'}^{p}$$

$$P(s - k + p', m - m', p - p') \times \text{coef. of } \xi^{p'}$$

$$\text{in } \exp[kD][(kA)^{m'}/m'!]\left(\sum_1^\infty j\xi^j\right)^{m'}, \tag{4.36}$$

which suggests the solution

$$P(s, m, p) = \exp[(p + s - 1)D] \frac{1}{\xi^p} \frac{1}{m!}$$

$$\times \left[(p+s)A \frac{\xi}{(1-\xi)^2}\right]^m, \tag{4.37}$$

where we have already used the starting point of the induction procedure:

$s + p = 1$, which implies $s = 1$, $p = m = 0$, for which $P(1, 0, 0) = 1$.

The lemma follows from (4.28), (4.33), (4.35), and (4.37). We finally prove the CP. From (4.23) we get

$$J_m \leq m! \sum_{k=1}^{\infty} \sum_{\gamma'(m-1)} (m-1)!$$

$$\times \int P^k_{xy}(d\omega)\, dx\, d\omega^{\gamma'}\, |z|^{q'+k}$$

$$\times \sum_{r=0}^{\infty} |z|^r \sum_{\delta(r)} \int d_+\omega^\delta\, |D_{(\omega,k;\omega^{\gamma'})} g(\omega^\delta)|. \tag{4.38}$$

Now

$$D_{(\omega,k;\omega^{\gamma'})} g(\omega^\delta) = D_{(\omega,k)} g(\omega^{\gamma'+\delta}) = \tilde\varphi_{(\omega,k)}(\omega^{\gamma'+\delta})$$

and $\int P^k_{xy}(d\omega)\, dx = 1$. Therefore

$$J_m \leq m!\,(m-1)! \sum_{k=1}^{\infty} \sum_{q'=m-1}^{\infty} \sum_{r=0}^{\infty} |z|^{k+q'+r} \times \sum_{\gamma'(m-1,q')} \sum_{\delta(r)} \sup_{(\omega,k)} \int d\omega^{\gamma'}\, d_+\omega^{\delta}\, |\tilde{\varphi}_{(\omega,k)}(\omega^{\gamma'+\delta})|. \tag{4.39}$$

We substitute the bound (4.26) in (4.39) and obtain after some straightforward algebra:

$$J_m \leq m! \left[\frac{A\xi}{(1-\xi)^2}\right]^{m-1} \frac{R}{1-\xi} \sum_{t=m}^{\infty} \left(\frac{|z|}{R}\right)^t t^{m-1} \times (1-\xi^{t-m+1}), \tag{4.40}$$

where the last series is absolutely convergent for any $|z| < R$.

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Two-Photon Ionization of Atomic Hydrogen. II*

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(Received 24 August 1964)

This paper contains a generalization of results described in previous work. A general formula is given for the total cross section for two-photon ionization of a hydrogenic state. An implicit method for evaluating the second-order radial matrix elements that occur in this expression is described in detail. Numerical results were obtained for the states with principal quantum numbers $n = 1$ through 5. It is concluded that, when both one-photon and two-photon ionization are energetically possible, the effect of the latter may be expressed as an intensity-dependent correction to the Gaunt factor which may therefore be written as $G = g_1 + \zeta I \lambda^3 g_2$. Here g_1 is the usual Gaunt factor, I is the intensity of the light in W cm^{-2}, λ is the wavelength in cm, g_2 is a dimensionless factor of order unity, and ζ is a constant given by $\zeta = 0.1504$ W^{-1} cm^{-1}. Graphs of g_2 are given as a function of electron energy.

These results do not include the effect of three-photon processes, which can also contribute to the first-order intensity-dependent correction to the Gaunt factor as a result of interference between the first- and third-order amplitudes.

I. INTRODUCTION

THE work described in this paper is a continuation and a generalization of that described in a previous paper,[1] hereinafter referred to as I. It is motivated by a desire to calculate the two-photon contribution to the absorption coefficient for optical radiation traversing a hydrogenic gas. For this reason, only total cross sections rather than differential cross sections are considered. A general formula for the total cross section for two-photon ionization of a hydrogenic state described by principal and orbital quantum numbers (n, l) is given in Sec. II.

In Sec. III it is shown how to generalize the method of calculating second-order matrix elements described in Sec. 3 of I so as to be able to compute such matrix elements for photon energies above the one-photon ionization threshold and for all possible initial and intermediate states.

The analysis described in Sec. III enables one to specify unique mathematical procedures for computing two-photon cross sections. In Sec. IV the computational technique is described in detail and the results of some numerical calculations are given.

Above the one-photon threshold, the two-photon cross sections are smooth functions of the incident frequency. This fact enables one to infer, from the results of Sec. IV, a two-photon correction to the well-known Kramers–Gaunt approximation for one-photon ionization of hydrogenic states by optical radiation. The result is given in Sec. V; it can be expressed in the form of an intensity-dependent Gaunt factor which is applicable when both one-photon and two-photon ionization are energetically possible.

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$$J_m \leq m!\,(m-1)! \sum_{k=1}^{\infty} \sum_{q'=m-1}^{\infty} \sum_{r=0}^{\infty} |z|^{k+q'+r} \times \sum_{\gamma'(m-1,q')} \sum_{\delta(r)} \sup_{(\omega,k)} \int d\omega^{\gamma'}\, d_+\omega^{\delta}\, |\tilde{\varphi}_{(\omega,k)}(\omega^{\gamma'+\delta})|. \tag{4.39}$$

We substitute the bound (4.26) in (4.39) and obtain after some straightforward algebra:

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II. TOTAL CROSS SECTION FOR TWO-PHOTON IONIZATION

In I, a general expression for the differential cross section per unit intensity, for a hydrogenic state described by quantum numbers (n, l, m), was derived [cf., Eqs. (10)–(13) of I].

In order to derive the total cross section, one must first integrate this expression over the solid angle, making use of the orthonormality of the spherical harmonic $Y_{lm}(\beta, \alpha)$. Next, one must average over the magnetic quantum numbers, making use of the relations

$$(2l+1)^{-1}\sum_{m=-l}^{l} m^2 = \frac{1}{3}\,l(l+1), \tag{1}$$

$$(2l+1)^{-1}\sum_{m=-l}^{l} m^4 = \frac{1}{15}\,l(l+1)(3l^2+3l-1). \tag{2}$$

After some burdensome algebra, one obtains the following expression for the total cross section per unit intensity for a hydrogenic state described by quantum numbers (n, l)

$$\frac{\sigma_{nl}}{I} = \frac{2\pi^2\alpha}{15I_0}E_p a^2\left\{\frac{2(l+1)(l+2)}{(2l+3)(2l+1)}|P^{nl}_{l+1,l+2}|^2 + \frac{2l(l-1)}{(2l-1)(2l+1)}|P^{nl}_{l-1,l-2}|^2 + \frac{(l+1)(4l^2+8l+5)}{(2l+1)^2(2l+3)}|P^{nl}_{l+1,l}|^2 + \frac{l(4l^2+1)}{(2l+1)^2(2l-1)}|P^{nl}_{l-1,l}|^2\right\}. \tag{3}$$

In this expression, I is the incident intensity in watts per square centimeter, α is the fine structure constant, I_0 is 7.019×10^{16} W/cm^2, E_p is the dimensionless photon energy in multiples of $me^4/\hbar^2$, and a is the Bohr radius. One has

$$2\pi^2\alpha a^2/15I_0 = 3.831 \times 10^{-36}\ \text{cm}^4/\text{W}. \tag{4}$$

The quantities $P^{nl}_{\lambda L}$ are dimensionless second-order matrix elements, given by

$$P^{nl}_{\lambda L} = \lim_{\epsilon\to 0}\sum_{\nu=\lambda+1}^{\infty}\frac{\langle R^c_L(k,r)|\,r\,|R_{\nu\lambda}(r)\rangle\langle R_{\nu\lambda}(r)|\,r\,|R_{nl}(r)\rangle}{(E_n - i\epsilon) - E_\nu + E_p}. \tag{5}$$

In Eq. (5), ν, λ are the principal and orbital quantum numbers of the intermediate states and L is the angular momentum quantum number of the final (continuum) state. The summation includes an integration over those intermediate states that lie in the continuum. The normalization of the various radial functions has been defined in Sec. 2 of I. The first and second radial matrix elements that appear in Eq. (5) are dimensionless multiples of $(\hbar^2/me^2)^{5/2}$ and $\hbar^2/me^2$, respectively. The energies that appear in the denominator are in dimensionless multiples of $me^4/\hbar^2$.

Equation (5) differs from Eq. (14) of I only in the presence of the small parameter ϵ. This parameter may be ignored provided that one is interested only in the two-photon cross section for photon energies below the one-photon ionization threshold. However, it is essential to include the limiting process on ϵ if one wishes to evaluate the matrix element (5) for photon energies above the one-photon threshold.[2] The way in which the inclusion of ϵ leads to an unambiguous evaluation of the second-order matrix element is described in the next section.

III. METHOD OF CALCULATING SECOND-ORDER MATRIX ELEMENTS

As an obvious generalization of Eq. (27) of I, one defines the quantity

$$U^n_{\lambda L}(r, E_p) = \lim_{\epsilon\to 0}\sum_{\nu=\lambda+1}^{\infty}\frac{rR_{\nu\lambda}(r)\int_0^\infty R_{\nu\lambda}(r')R^c_L(k_\epsilon, r')r'^3\,dr'}{(E_n - i\epsilon) - E_\nu + E_p}. \tag{6}$$

Hence one has

$$P^{nl}_{\lambda L}(E_p) = \int_0^\infty R_{nl}(r)U^n_{\lambda L}(r, E_p)r^2\,dr. \tag{7}$$

Because of the structure of the bound hydrogenic radial functions, the quantity $P^{nl}_{\lambda L}$ can always be expressed as a sum of derivatives of the Laplace transform of $U^n_{\lambda L}$, which is defined by

$$S^n_{\lambda L}(p, E_p) = \int_0^\infty U^n_{\lambda L}(r, E_p)e^{-pr}\,dr. \tag{8}$$

It is clear that the derivatives of these functions will be required only at the point $p = 1/n$.

Now, the functions $rR_{\nu\lambda}(r)$ satisfy the radial Schrödinger equation

$$\frac{1}{2}\frac{d^2}{dr^2}[rR_{\nu\lambda}(r)] + \left[\frac{1}{r} - \frac{\lambda(\lambda+1)}{2r^2}\right]rR_{\nu\lambda}(r) = -E_\nu rR_{\nu\lambda}(r). \tag{9}$$

[2] The problem that is involved here is just that of calculating transitions by second-order time-dependent perturbation theory when transitions can also occur in first order. It is discussed, for instance, in L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., pp. 202–205. An alternative discussion is given in W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, New York, 1954), 3rd ed., pp. 163–172. It is clear from the latter that the addition of a negative imaginary part to the energy of the initial state is simply a consequence of the fact that this state is decaying in time as a result of the interaction with the radiation field.

Hence, by means of the closure condition, one finds that $U_{\lambda L}(r, E_p)$ satisfies

$$\left[(E_n - i\epsilon) + E_p + \frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{r} - \frac{\lambda(\lambda+1)}{2r^2}\right]U_{\lambda L}(r, E_p) = R_L^c(k_e, r)r^2. \quad (10)$$

If one takes the Laplace transform of this equation, one finds that $S^n_{\lambda L}(p, E_p)$ satisfies

$$\left[(E_n - i\epsilon) + E_p + \frac{1}{2}p^2\right]\frac{d^2S^n_{\lambda L}}{dp^2} + (2p-1)\frac{dS^n_{\lambda L}}{dp} + \left[1 - \frac{1}{2}\lambda(\lambda+1)\right]S^n_{\lambda L} = \int_0^\infty R_L^c(k_e, r)r^4e^{-pr}\,dr. \quad (11)$$

If $\lambda = 1$, the term in $S^n_{\lambda L}$ vanishes so that Eq. (11) is effectively of first order and can be solved for $dS^n_{\lambda L}/dp$ by means of a single boundary condition. This was the case in I where the only intermediate states that were required were p states. However, a first-order differential equation can be derived for *any* value of λ. To see this, one differentiates Eq. (11) to obtain

$$\left[(E_n - i\epsilon) + E_p + \frac{1}{2}p^2\right]\frac{d^3S^n_{\lambda L}}{dp^3} + (3p-1)\frac{d^2S^n_{\lambda L}}{dp^2} + \left[3 - \frac{1}{2}\lambda(\lambda+1)\right]\frac{dS^n_{\lambda L}}{dp} = -\int_0^\infty R_L^c(k_e, r)r^5e^{-pr}\,dr. \quad (12)$$

Equation (12) is of first order in $d^2S^n_{\lambda L}/dr^2$ if $\lambda = 2$. By differentiating Eq. (12) in turn, one can find an effectively first-order equation for $\lambda = 3$, and so on. One can also find a first-order equation for $\lambda = 0$ directly from Eq. (10). In this way, one finds that the *general* form of the first-order equation for $d^\lambda S^n_{\lambda L}(r, E_p)/dp^\lambda$ is

$$\left[(E_n - i\epsilon) + E_p + \frac{1}{2}p^2\right]\frac{d^{\lambda+1}S^n_{\lambda L}}{dp^{\lambda+1}} + [(\lambda+1)p - 1]\frac{d^\lambda S^n_{\lambda L}}{dp^\lambda} = (-1)^{\lambda+1}\int_0^\infty R_L^c(k_e, r)r^{\lambda+3}e^{-pr}\,dr. \quad (13)$$

As the dipole selection rules require that $L = \lambda \pm 1$, the right-hand side of Eq. (13) may always be evaluated by differentiating Eq. (15) of I either once or three times with respect to p. Of course, the solution of Eq. (13) does not determine the values of derivatives of $S^n_{\lambda L}$ that are of lower order than λ, but it turns out that such derivatives are never needed to evaluate the $P^{ni}_{\lambda L}$. The initial condition for Eq. (13) is an immediate consequence of the definition Eq. (8) and is that $S^n_{\lambda L}(p, E_p)$ and all its derivatives are finite for all p such that Re $p > 0$. Thus for $E_n + E_p < 0$, one can forget about the parameter ϵ and simply determine, from Eq. (13), a boundary value of $d^\lambda S^n_{\lambda L}/dp^\lambda$ at the positive value of p for which the coefficient of $d^{\lambda+1}S^n_{\lambda L}/dp^{\lambda+1}$ vanishes.

Above the one-photon threshold, when $E_n + E_p > 0$, one must proceed as follows. Setting the coefficient of the first term in Eq. (13) equal to zero gives

$$\tfrac{1}{2}p^2 = -a + i\epsilon, \qquad a > 0. \quad (14)$$

Hence

$$p = \pm[i(2a)^{\frac{1}{2}} + \epsilon(2a)^{-\frac{1}{2}}], \quad (15)$$

to first order in ϵ. In order to have Re $p > 0$, one must choose the positive sign in Eq. (15). This determines a starting value of p that is infinitesimally close to the *positive imaginary* axis and in the *first* quadrant of the complex plane.

One may conclude that the parameter ϵ may be dropped provided one states as a boundary condition for Eq. (13) that $S^n_{\lambda L}(p, E_p)$ and all its derivatives are finite for all p on the positive real or positive imaginary axis. This condition enables one always to find a boundary value of $d^\lambda S^n_{\lambda L}/dp^\lambda$ at a value of p for which the coefficient of $d^{\lambda+1}S^n_{\lambda L}/dp^{\lambda+1}$ vanishes, since this value of p can be chosen so that the quantity $d^{\lambda+1}S^n_{\lambda L}/dp^{\lambda+1}$ is finite.

The conclusion of the last paragraph may be put in another way. The condition that the solution of Eq. (13) be analytic at an initial value of p [chosen so as to be in the first quadrant of the complex plane and to make the coefficient of the first term in Eq. (13) vanish] is sufficient to select a unique solution. It follows that all the other (incorrect) solutions of Eq. (13) are *not* analytic at the initial value of p. This point must be kept in mind in designing the strategy for a numerical solution.

IV. THE NUMERICAL SOLUTION

The differential equation (13) may be restated as

$$(p^2 - \alpha^2)(dy_{\lambda,L}/dp) + 2[(\lambda+1)p - 1]y_{\lambda,L} = 2F_{\lambda,L}(p, k), \quad (16)$$

where

$$y_{\lambda,L} = d^\lambda S^n_{\lambda,L}/dp^\lambda, \quad (17)$$

$$F_{\lambda,L}(p, k) = A_L(k) \frac{d^{\lambda-L+2}}{dp^{\lambda-L+2}} \times \left\{ \frac{\exp[-(2/k) \operatorname{arccot}(p/k)]}{(p^2 + k^2)^{L+1}} \right\}, \quad (18)$$

$$A_L(k) = \frac{(-2)^{L+1}}{(1 - e^{-2\pi/k})^{\frac{1}{2}}} \times [(1 + k^2)(1 + 4k^2) \cdots (1 + L^2k^2)]^{\frac{1}{2}}, \quad (19)$$

$$\alpha^2 = n^{-2} - 2E = \tfrac{1}{2}[n^{-2} - k^2], \quad (20)$$

$$k^2 = 4E - n^{-2}. \quad (21)$$

In Eqs. (20) and (21), and henceforth, the subscript on E_p is dropped.

Solutions for $y_{\lambda,L}$ and its higher derivatives are to be obtained at $p = 1/n$ subject to the condition that $y_{\lambda,L}$ is analytic at the point $p = \alpha$. By definition, α is positive real or on the positive imaginary axis. It is characteristic of the problem that no such solution exists when α is the reciprocal of a positive integer greater than λ. The corresponding values of E are either unphysical in that they are below the two-photon ionization threshold, or they correspond to the resonance peaks in the two-photon cross section which, as pointed out in I, must be treated by means of the "strong signal" approach.

It is to be recalled that

$$\lambda = l \pm 1 \not< 0, \qquad l < n \quad (22)$$

$$L = \lambda \pm 1 \not< 0, \quad (23)$$

and hence

$$\lambda - L + 2 = 1 \text{ or } 3. \quad (24)$$

At first glance, Eq. (16) appears to be quite innocent since it is a first-order linear differential equation with variable coefficients. The standard method of applying an appropriate integrating factor fails in this case, however, since the definite integrals so obtained fail to converge in the range of α's of interest.

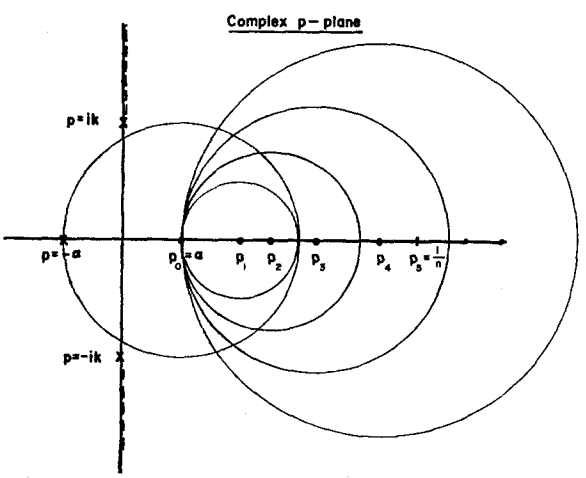

FIG. 1. Complex p plane for α real positive.

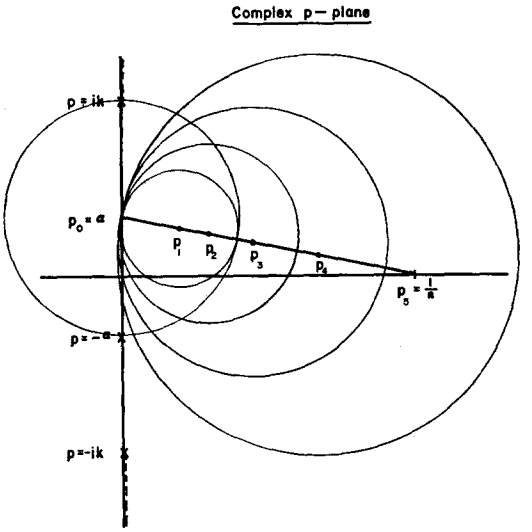

FIG. 2. Complex p plane for α pure imaginary.

A direct numerical integration of Eq. (16) will be effective for part of the range of interest but will fail when α is near the reciprocal of a positive integer greater than λ and p is near α, due to loss of significance in the evaluation of $dy_{\lambda,L}/dp$. To circumvent this, it is necessary to develop a Taylor series for $y_{\lambda,L}$ about the point $p = \alpha$.

Since Taylor series would be required in any case, it was decided to develop a method of solution based on Taylor series alone. The computations were readily organized from this point of view and good accuracy control could be retained. This is the approach described below.

A. Characteristics of the Solution

Figures 1 and 2 show the location of the singularities, branch points and cuts for solutions of Eq. (16). There is a singularity at $p = -\alpha$ due to the form of the differential equation. There are poles and branch points at $p = \pm ik$ due to the properties of $F_{\lambda,L}(p, k)$.

Since k is always real the corresponding singularities and branch points always appear on the imaginary axis. On the other hand, α may take on either real or imaginary values. α is real for

$$1/4n^2 \leq E \leq 1/2n^2,$$

(below the one-photon threshold)

and pure imaginary for

$$1/2n^2 \leq E$$

(above the one-photon threshold).

These two cases are illustrated in Figs. 1 and 2. The potential singularity at $p = +\alpha$ is suppressed by the choice of initial condition for $y_{\lambda,L}$ at this point.

The strategy for solution is to form an initial Taylor series about the point $p_0 = \alpha$. The radius of convergence of this series will be limited by the singularities at $p = \pm ik$ for

$$1/4n^2 \leq E \leq 2/5n^2,$$

by the singularity at $p = -\alpha$ for

$$2/5n^2 \leq E \leq 4/7n^2,$$

and by the singularity at $p = +ik$ for

$$4/7n^2 \leq E.$$

This series is evaluated at a point p_1 on the line connecting $p_0 = \alpha$ to $p = 1/n$. Experience has shown that evaluation at half the radius of convergence results in a loss of less than four digits of accuracy in the sum.

At this point it is essential to keep in mind that the solution to Eq. (16) that one is evaluating is only an approximation to the correct solution, since one is keeping only a finite number of terms in the Taylor series and there are, in any case, round-off errors in the computer operations. Consequently, recalling the argument of the last paragraph of Sec. III, one must treat the point $p_0 = +\alpha$ as a singularity for all Taylor series expansions subsequent to the first. If this is not done, the small computational errors arising in the first expansion will be amplified in subsequent expansions and may completely obscure the desired solution. Thus, the radius of convergence of all the Taylor series expansions subsequent to the first is limited by the point $p_0 = +\alpha$.

Now a new Taylor series is formed about the point $p = p_1$. This new series is used to evaluate the solution at a point p_2 (see Figs. 1 and 2). The process is continued until the solution can be evaluated at $p = 1/n$ which is the desired result. It is to be noted that if the individual terms of the most recent series are retained at each stage, the desired derivatives can be formed at the end by operations on this series. They can, of course, also be obtained through successive differentiation of Eq. (16) at the expense of some analytical work.

It is a fairly straightforward matter to evaluate the number of Taylor series expansions that are required to obtain the solution at $p = 1/n$. Let M denote the required number of expansions, r the fraction of the radius of convergence that is used each time, and the symbol $[[x]]$ the largest integer less than x. One finds that

$$M = 2 + \left[\left[\frac{\log\left\{\frac{1}{r}\left(\frac{1 - n\,|\alpha|}{1 + n\,|\alpha|}\right)^{\frac{1}{2}}\right\}}{\log(1 + r)}\right]\right],$$

$$\frac{1}{4n^2} \leq E \leq \frac{2}{5n^2}, \tag{25}$$

$$M = 2 + \left[\left[\frac{\log\left\{\frac{1}{2r}\left(\frac{1 - n\,|\alpha|}{n\,|\alpha|}\right)\right\}}{\log(1 + r)}\right]\right],$$

$$\frac{2}{5n^2} \leq E \leq \frac{1}{2n^2}, \tag{26}$$

$$M = 2 + \left[\left[\frac{\log\left\{\frac{1}{2r}\frac{(1 + n^2\,|\alpha|^2)^{\frac{1}{2}}}{n\,|\alpha|}\right\}}{\log(1 + r)}\right]\right],$$

$$\frac{1}{2n^2} \leq E \leq \frac{4}{7n^2}, \tag{27}$$

$$M = 2 + \left[\left[\frac{\log\left\{\frac{1}{r}\frac{(1 + n^2\,|\alpha|^2)^{\frac{1}{2}}}{(1 + 2n^2\,|\alpha|^2)^{\frac{1}{2}} - n\,|\alpha|}\right\}}{\log(1 + r)}\right]\right],$$

$$\frac{4}{7n^2} \leq E. \tag{28}$$

It is apparent that, generally, only a modest number of expansions is required since M increases only logarithmically as $E \to 1/2n^2$ (i.e., $\alpha \to 0$). In the present calculations it was found satisfactory to take $r = 0.5$. As $E \to \infty$, one finds from Eq. (28) that $M \to 5$.

It is clear on physical grounds that difficulties are to be anticipated in the perturbation theoretic evaluation of the two-photon cross section as the photon energy approaches the one-photon threshold from below. This is because the resonances in the two-photon cross section become increasingly close to one another. It is apparent from Eqs. (26) and (27) that as the photon energy approaches the one-photon threshold from either above or below the number of expansions required tends logarithmically to infinity. This is because the radius of convergence of each Taylor series tends to zero. Moreover, as $\alpha \to 0$, a small error in the initial expansion can cause an increasingly large error in the final value of y. For these reasons, it was decided not to carry out the numerical calculations for $|\alpha| < 0.06$. The maximum number of terms required in any Taylor

series was 100 and the maximum number of expansions required was 11.

It is shown in the following sections that this process can be completely automated. The series are formed numerically by a computer program at each stage rather than from explicit analytic representations. The total process may be viewed as numerical analytic continuation.

Numerical results from a computer program for the RCA 601 computer at RCA Laboratories are given in Sec. IVE.

B. Series Solution of Eq. (16)

An arbitrary point p_0 in the complex p plane is considered and it is assumed that $y_{\lambda,L}(p_0) = y_0$ is known. The complex variable ξ is defined as

$$\xi = p - p_0 \tag{29}$$

and the Taylor series for $F_{\lambda,L}$

$$F_{\lambda,L}(p, k) = \sum_{m=0}^{\infty} b_m \xi^m \tag{30}$$

is considered as known. An algorithm for its generation is described in Sec. IVC.

Now set

$$y_{\lambda,L}(p) = \sum_{m=0}^{\infty} a_m \xi^m. \tag{31}$$

Substitution into Eq. (16) leads to

$$\begin{aligned}\sum_{m=2}^{\infty} &\{(p_0^2 - \alpha^2)(m+1)a_{m+1} + 2[(\lambda + 1 + m)p_0 - 1]a_m \\ &+ (m + 2\lambda + 1)a_{m-1} - 2b_m\}\xi^m \\ &+ \{2p_0 a_1 + 2(p_0^2 - \alpha^2)a_2 + 2(\lambda + 1)a_0 \\ &+ 2[(\lambda + 1)p_0 - 1]a_1 - 2b_1\}\xi \\ &+ \{(p_0^2 - \alpha^2)a_1 + 2[(\lambda + 1)p_0 - 1]a_0 - 2b_0\} \equiv 0. \end{aligned} \tag{32}$$

Hence, when $p_0 \neq \pm\alpha$,

$$a_0 = y_0, \tag{33}$$

$$a_1 = 2\{b_0 - [(\lambda + 1)p_0 - 1]a_0\}/(p_0^2 - \alpha^2), \tag{34}$$

and

$$\begin{aligned} a_{m+1} &= \{2b_m - 2[(\lambda + m + 1)p_0 - 1]a_m \\ &- [m + 2\lambda + 1]a_{m-1}\}[(m+1)(p_0^2 - \alpha^2)]^{-1}, \quad m \geq 1. \end{aligned} \tag{35}$$

The coefficients of the Taylor series are hence recursively determined.

At the initial point, $p_0 = \alpha$, a_0 is obtained from Eq. (16) and the condition that $dy_{\lambda,L}/dp$ is finite at this point

$$a_0 = b_0/[(\lambda + 1)\alpha - 1]. \tag{36}$$

Consideration of Eq. (32) with $p_0 = \alpha$ leads to

$$a_{m+1} = \frac{2b_{m+1} - [m + 2\lambda + 2]a_m}{2[(\lambda + m + 2)\alpha - 1]}, \quad m \geq 0. \tag{37}$$

In the computational procedure, it turns out that certain scaling problems are avoided if the quantities

$$\alpha_m = a_m \xi^m, \tag{38}$$

$$\beta_m = b_m \xi^m, \tag{39}$$

are generated rather than a_m and b_m.

The corresponding recursion relations are, for $p_0 \neq \pm\alpha$

$$\alpha_0 = y_0, \tag{40}$$

$$\alpha_1 = \frac{2\beta_0 - 2[(\lambda + 1)p_0 - 1]\alpha_0}{p_0^2 - \alpha^2}\xi, \tag{41}$$

$$\begin{aligned}\alpha_{m+1} &= \{2\beta_m - 2[(m + \lambda + 1)p_0 - 1]\alpha_m \\ &- \xi[m + 2\lambda + 1]\alpha_{m-1}\}[(m+1)(p_0^2 - \alpha^2)]^{-1}\xi, \quad m \geq 1. \end{aligned} \tag{42}$$

Also, when $p_0 = \alpha$

$$\alpha_0 = \beta_0/[(\lambda + 1)\alpha - 1], \tag{43}$$

$$\alpha_{m+1} = \frac{2\beta_{m+1} - \xi[m + 2\lambda + 2]\alpha_m}{2[(\lambda + m + 2)\alpha - 1]}, \quad m \geq 0. \tag{44}$$

The recursion relation (44) exhibits directly the lack of existence of an analytic solution when α is the reciprocal of an integer larger than λ.

In the computer program the quantities α_m are generated recursively along with the β_m and stored.

C. Taylor Series for $F_{\lambda,L}(p, k)$

One now considers the function

$$G_L(p, k) = \frac{\exp[-(2/k)\operatorname{arccot}(p/k)]}{(p^2 + k^2)^{L+1}}. \tag{45}$$

One differentiates with respect to p to obtain

$$G_L^{(1)}(p, k) = \{2[1 - (L+1)p]\}G_L(p, k)/(p^2 + k^2). \tag{46}$$

Continued differentiation of Eq. (46) leads to the general relation

$$\begin{aligned}(p^2 + k^2)G_L^{(n+1)} &= 2[1 - (L + 1 + n)p]G_L^{(n)} \\ &- n(2L + n + 1)G_L^{(n-1)}. \end{aligned} \tag{47}$$

This furnishes a basis for generating the Taylor series for $F_{\lambda,L}(p, k)$ about any point $p = p_0$.

Two situations can be distinguished, namely, $\lambda + 2 - L = 1$ and $\lambda + 2 - L = 3$. When $\lambda + 2 - L = 1$, one has

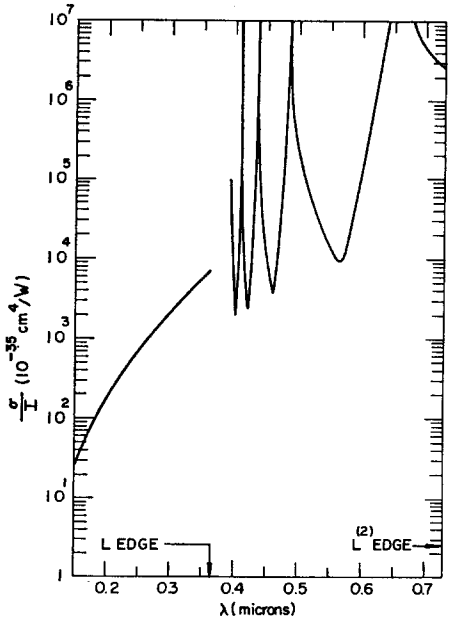

FIG. 3. Two-photon cross section for H, $n = 2$.

$$F_{\lambda,L}(p, k) = A_L(k)\, dG_L(p, k)/dp = A_L(k) \sum_{n=0}^{\infty} \frac{G_L^{(n+1)}(p_0)}{n!} \xi^n = \sum_{m=0}^{\infty} b_m \xi^m = \sum_{m=0}^{\infty} \beta_m. \tag{48}$$

From Eq. (47) one has

$$(p_0^2 + k^2)G_L^{(n+2)} = 2[1 - (L + 2 + n)p_0]G_L^{(n+1)} - (n + 1)(2L + n + 2)G_L^{(n)}, \tag{49}$$

so that

$$b_{m+1} = \frac{1}{p_0^2 + k^2}\left\{\frac{2[1 - (L + 2 + m)p_0]}{m + 1} b_m - \frac{2L + m + 2}{m} b_{m-1}\right\}, \tag{50}$$

and

$$\beta_{m+1} = \frac{\xi}{p_0^2 + k^2}\left\{\frac{2[1 - (L + 2 + m)p_0]}{m + 1} \beta_m - \xi \frac{2L + m + 2}{m} \beta_{m-1}\right\}, \tag{51}$$

with

$$\beta_0 = A_L(k)G_L^{(1)}(p_0), \tag{52}$$

$$\beta_1 = \xi A_L(k)G_L^{(2)}(p_0), \tag{53}$$

being generated from Eqs. (45)–(47).

When $\lambda + 2 - L = 3$, one has

$$F_{\lambda,L}(p, k) = A_L(k)(d^3/dp^3)G_L(p, k) = A_L(k) \sum_{n=0}^{\infty} \frac{G_L^{(n+3)}(p_0)}{n!} \xi^n = \sum_{m=0}^{\infty} b_m \xi^m = \sum_{m=0}^{\infty} \beta_m. \tag{54}$$

As before

$$(p_0^2 + k^2)G_L^{(n+4)} = 2[1 - (L + 4 + n)p_0]G_L^{(n+3)} - (n + 3)(2L + n + 4)G_L^{(n+2)}, \tag{55}$$

which leads to

$$b_{m+1} = \frac{1}{p_0^2 + k^2}\left\{\frac{2[1 - (L + 4 + m)p_0]}{(m + 1)} b_m - \frac{(m + 3)(2L + m + 4)}{m(m + 1)} b_{m-1}\right\}, \tag{56}$$

$$\beta_{m+1} = \frac{\xi}{p_0^2 + k^2}\left\{\frac{2[1 - (L + 4 + m)p_0]}{m + 1} \beta_m - \xi \frac{(m + 3)(2L + m + 4)}{m(m + 1)} \beta_{m-1}\right\}, \tag{57}$$

with

$$\beta_0 = A_L(k)G_L^{(3)}(p_0), \tag{58}$$

$$\beta_1 = \xi A_L(k)G_L^{(4)}(p_0), \tag{59}$$

being generated from Eqs. (45)–(47).

D. Calculation of the $P_{\lambda L}^{nl}$

If one now makes use of Eqs. (7) and (8), and the well-known general expression for the $R_{nl}(r)$, one easily finds that

$$P_{\lambda L}^{nl} = \frac{1}{(2l + 1)!}\left[\frac{4(n + l)!}{(n - l - 1)!n^4}\right]^{\frac{1}{2}}\left(\frac{2}{n}\right)^l (-1)^l \times \left\{F\left[-(n - l - 1), (2l + 2), -\frac{2}{n}\frac{d}{dp}\right] \times \frac{d^{l-\lambda+2}y_{\lambda,L}}{dp^{l-\lambda+2}}\right\}_{p=1/n}, \tag{60}$$

where F is the confluent hypergeometric function

$$F(\alpha, \beta, x) = 1 + \frac{\alpha}{\beta \cdot 1!} x + \frac{\alpha(\alpha + 1)}{\beta(\beta + 1) \cdot 2!} x^2 + \cdots. \tag{61}$$

One can now find the cross section per unit intensity per electron for each subshell from Eq. (3), and the cross section per unit intensity per electron for each shell from

$$\sigma_n = \frac{1}{n^2} \sum_{l=0}^{n-1} (2l + 1)\sigma_{nl}. \tag{62}$$

E. Numerical Results

The cross sections per unit intensity were calculated in detail as a function of wavelength for the states with $n = 2$ and $n = 3$. The results are shown in Figs. 3 and 4, respectively. One notes the expected resonant structure of the two-photon cross section for photon energies below the one-photon threshold and the smooth behavior (varying approximately as λ^6) for photon energies above this threshold. Additional calculations, for photon energies above the one-photon threshold only, were carried out for $n = 1$, 3, and 5.

V. TWO-PHOTON CORRECTION TO THE GAUNT FACTOR

On the basis of the numerical calculations described in Sec. IV, one may induce the following result:

When both one-photon and two-photon ionization are energetically possible, the average cross section (in square centimeters) per electron in the n shell, for a hydrogenic atom with nuclear charge Z, for ionization by light of wavelength λ(cm) and intensity I (W/cm^2) is

$$\sigma_n(Z, \lambda) = (1.045 \times 10^{-2})[Z^4 n^{-5} \lambda^3 g_1 + I(I_0^{-1}\lambda_0^{-3}) Z^4 n^{-5} \lambda^6 g_2]. \quad (63)$$

The first term in Eq. (63) is the well known Kramers–Gaunt formula; g_1, called the Gaunt factor, is a number which depends slightly on n and λ but is of order unity.[3] The second term is the result of the present investigation; the precise value of the numerical factor g_2, like that of g_1, depends slightly on n and λ, but it is also of order unity. I_0 is the atomic unit of itensity (7.019×10^{16} W/cm^2) and λ_0 is the atomic unit of wavelength (455.88 Å). The induction of the second term from the numerical calculations is simplified by the fact that one expects an n^{-5} dependence, just as in the first term, since this clearly arises from the energy density of electron states in the hydrogen atom. Furthermore, once the λ dependence has been established, the Z dependence follows from the general structure of the perturbation theory result [cf. Eq. (3) of I]. Thus, the numerical calculations are required only to determine the λ dependence and a numerical factor.

The above result may be expressed more simply by saying that, at high intensities, one should use an intensity-dependent Gaunt factor given by

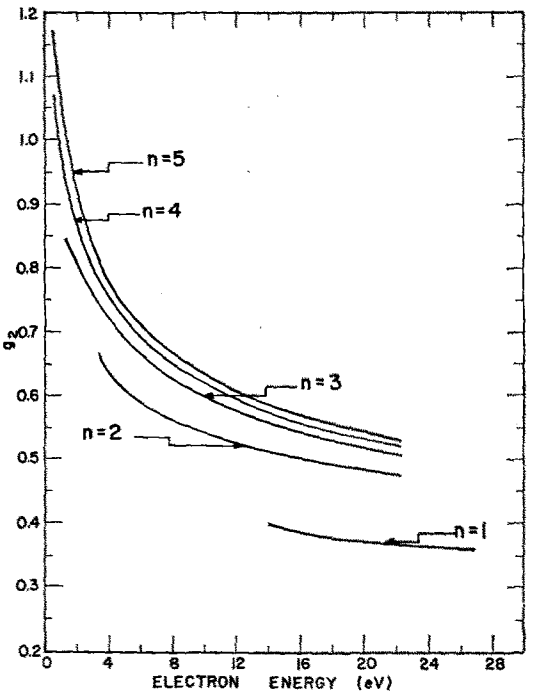

FIG. 5. The numerical factor g_2 as a function of the energy of the electrons produced by two-photon ionization for photon energies above the one-photon threshold.

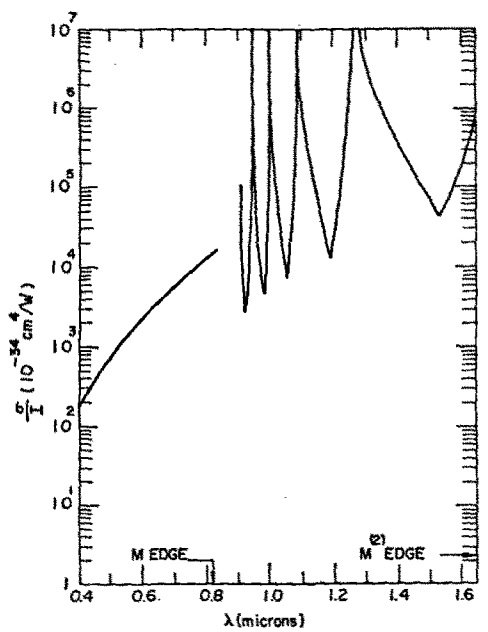

FIG. 4. Two-photon cross section for H, $n = 3$.

[3] For a statement of the Kramers–Gaunt formula and some indication of its application to astrophysical problems, see, for instance, C. W. Allen, *Astrophysical Quantities* (University of London Press, London, 1963), 2nd ed., pp. 90–91; M. Schwartzschild, *Structure and Evolution of the Stars* (Princeton University Press, Princeton, New Jersey, 1958), pp. 63–64. For the original papers, see H. A. Kramers, Phil. Mag. **46**, 836 (1923); J. A. Gaunt, Phil. Trans. **A229**, 163 (1930). For some of the subsequent work see footnote 28 of I and H. Mayer, Los Alamos Report LA-647 (March 1948); W. J. Karzas and R. Latter, Astrophys. J. Suppl. **6**, 167 (1961).

$$G(I) = g_1 + \zeta I \lambda^3 g_2, \tag{64}$$

where g_1 is the usual Gaunt factor, of order unity, and g_2 is a similar factor also of order unity, shown in Fig. 5. The constant ζ is given by

$$\zeta = I_0^{-1}\lambda_0^{-3} = 0.1504\ \mathrm{W}^{-1}\ \mathrm{cm}^{-1}. \tag{65}$$

The result expressed by Eqs. (64) and (65) enables one to make quantitative statements regarding the magnitude of two-photon effects for the absorption of laser radiation by hot plasmas.

The results shown in Fig. 5 suggest that g_2 is probably of order unity for all n, with λ in the optical range. It follows that the first-order intensity-dependent correction to the Gaunt factor is practically independent of both the effective nuclear charge Z and the principal quantum number n. Consequently, for a hot gas, this correction is independent of the temperature of the gas and should not depend very much on the atomic constituents either. Further, since one can derive the cross section for free–free absorption from that for bound–free absorption by simply replacing the density of states for a bound hydrogenic system by the density of states in the continuum,[4] it follows that Eqs. (64) and (65), with $g_2 = 1$, should be approximately valid also for the free–free transitions.

If one sets $g_2 = 1$ and $\lambda = 6943$ Å one finds, in the present approximation, that the Gaunt factor is increased by 1% at an intensity of approximately 2×10^{11} W/cm^2. However, this conclusion does not take into account the possibility of third-order processes. Some of these processes, consisting of the absorption of two photons and the induced emission of one photon, can lead to the same continuum states as the first-order process. Consequently, there is a term in the cross section arising from interference between first- and third-order amplitudes, which is linear in the intensity.[5] The results obtained by Rand, who has made an approximate calculation of free–free absorption at high intensities using methods quite different from those described in the present paper, suggest that the net first-order intensity dependent correction to the Gaunt factor is in fact negative.[6] However, the absolute magnitude of the correction is still determined in his theory by the ratio of $\zeta I \lambda^3$ to unity.

ACKNOWLEDGMENTS

The authors would like to thank Dr. Edward Gerjuoy for his interest and several useful discussions. Thanks are also due to John O'Neil for his efforts in programming the calculations.

[4] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms* (Academic Press Inc., New York, 1957), Sec. 78.

[5] S. Rand, (personal communication).

[6] S. Rand, Phys. Rev. **136**, B 231, (1964).

Use of Analytic Signals in Third- and Fourth-Order Coherence Functions*

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In this paper complex forms of the third- and fourth-order coherence functions are defined using analytic signals. The relations between the complex forms and the real forms are given in detail. It is shown how to use the complex forms in the solution of radiation problems. The quasimonochromatic approximation greatly simplifies the calculations and this simplification is discussed for radiation problems in terms of the complex forms. The paper concludes with a discussion of quasimonochromatic radiation from a modulated incoherent source representing, perhaps, a self-luminous turbulent region.

1. INTRODUCTION

IN order to describe electromagnetic fields with stationary statistical properties much attention has been given to the properties of the second-order moment called the mutual coherence function.[1] If $E_i^r(\mathbf{x}, t)$ is the field variation, the real form of the mutual coherence function $\mathcal{E}_{ik}^{rr}(\mathbf{x}_1, \mathbf{x}_2, \tau)$ is defined as

$$\mathcal{E}_{ik}^{rr}(\mathbf{x}_1, \mathbf{x}_2, \tau) = \langle E_i^r(\mathbf{x}_1, t + \tau) E_k^r(\mathbf{x}_2, t) \rangle, \quad (1)$$

where the brackets, $\langle\ \rangle$, indicate a time average, and the subscripts indicate vector components. It has proved convenient for the solution of radiation problems, however, to also introduce a complex form of the mutual coherence function, $\mathcal{E}_{ik}(\mathbf{x}_1, \mathbf{x}_2, \tau)$, defined as

$$\mathcal{E}_{ik}(\mathbf{x}_1, \mathbf{x}_2, \tau) = \langle E_i(\mathbf{x}_1, t + \tau) E_k^*(\mathbf{x}_2, t) \rangle, \quad (2)$$

where $E_i(\mathbf{x}, t)$ is an analytic signal[1-3] [* indicates the complex conjugate], defined as

$$E_i(\mathbf{x}, t) = E_i^r(\mathbf{x}, t) + iE_i^i(\mathbf{x}, t), \quad (3)$$

$E_i^i(\mathbf{x}, t)$ being the Hilbert transform of $E_i^r(\mathbf{x}, t)$. Superscripts denote real and imaginary parts. [Care must be taken to properly define the manner of taking the limit in Eq. (2) and of defining the Hilbert transform since $E_i^r(\mathbf{x}, t)$ exists for all time. In the interests of continuity however, we defer this point until Sec. 2.]

Recently attention has been given to higher moments of the electromagnetic field and it is the purpose of this paper to consider a convenient complex form to associate with the real forms of the third- and fourth-order coherence functions,

$$T_{jkl}^{rrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3)$$

and

$$L_{jklm}^{rrrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4),$$

where

$$T_{jkl}^{rrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \langle E_j^r(\mathbf{x}_1, t) E_k^r(\mathbf{x}_2, t + \tau_2) E_l^r(\mathbf{x}_3, t + \tau_3) \rangle \quad (4)$$

and

$$L_{jklm}^{rrrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = \langle E_j^r(\mathbf{x}_1, t) E_k^r(\mathbf{x}_2, t + \tau_2) E_l^r(\mathbf{x}_3, t + \tau_3) E_m^r(\mathbf{x}_4, t + \tau_4) \rangle. \quad (5)$$

There are many reasons for introducing a complex analytic signal representation. In particular, the definition given in Eq. (3) is equivalent to the useful procedure of replacing a Fourier cosine representation (assuming for the moment that it exists; see Sec. 2 for a proper definition):

$$E_i^r(\mathbf{x}, t) = \int_0^\infty A_i(\mathbf{x}, \nu) \cos(-2\pi\nu t + \phi(\mathbf{x}, \nu))\, d\nu \quad (6)$$

by the exponential representation

$$E_i(\mathbf{x}, t) = \int_0^\infty A_i(\mathbf{x}, \nu) \exp[i(-2\pi\nu t + \phi(\mathbf{x}, \nu))]\, d\nu \quad (7)$$

(note the integral over ν is only over positive frequencies).

In the exponential representation it is easy to insure, for example, that the function $\hat{E}_i(\mathbf{x}, \nu) = A_i(\mathbf{x}, \nu) \exp[i\phi(\mathbf{x}, \nu)]$, which satisfies Helmholtz's equation [$\hat{E}_i$ is the Fourier transform of E_i], has the appropriate form for an outgoing spherical wave in the far field of a source; in an r, θ, α spherical coordinate system it is required that $\hat{E}_i(\mathbf{x}, \nu) \to f(\theta, \alpha, \nu)e^{ikr}$ as $r \to \infty$ ($k \equiv 2\pi\nu/c$).

If the third- and fourth-order coherence functions

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[1] M. Beran and G. B. Parrent, Jr., *Theory of Partial Coherence* (Prentice Hall, Inc., Englewood Cliffs, New Jersey, 1964).

[2] D. Gabor, J. Inst. Elec. Engrs. (London) 93, 429 (1946).

[3] M. Born and E. Wolf, *Principles of Optics* (Pergamon Press, Ltd., London, 1959).

are defined in terms of $E_i(\mathbf{x}, t)$ or $E_j^*(\mathbf{x}, t)$ rather than $E_i^r(\mathbf{x}, t)$, the Sommerfeld condition will thus be easily met. The problem that arises, however, is finding what combination of $E_i(\mathbf{x}_1, t_1)$ and $E_k^*(\mathbf{x}_2, t_2)$ will be most appropriate to use. In the second-order case it was natural to use $E_i(\mathbf{x}_1, t + \tau)$ at point $\mathbf{x}_1$ and the complex conjugate $E_k^*(\mathbf{x}_2, t)$ at point $\mathbf{x}_2$. [$E_i(\mathbf{x}_1, t)$ and $E_k^*(\mathbf{x}_2, t + \tau_2)$ could also of course have been used.] With this definition it may be shown that

$$\mathrm{Re}\,[\mathcal{E}_{ik}(\mathbf{x}_1, \mathbf{x}_2, \tau)] = 2\mathcal{E}_{ik}^{rr}(\mathbf{x}_1, \mathbf{x}_2, \tau), \tag{8}$$

where Re signifies the real part. Further, it follows that $\mathcal{E}_{ik}(\mathbf{x}_1, \mathbf{x}_2, \tau)$ is itself an analytic signal in the variable τ, that is,

$$\mathrm{Im}\,[\mathcal{E}_{ik}(\mathbf{x}_1, \mathbf{x}_2, \tau)] = \mathfrak{H}_\tau[\mathcal{E}_{ik}^{rr}(\mathbf{x}_1, \mathbf{x}_2, \tau)], \tag{9}$$

where Im denotes the imaginary part and $\mathfrak{H}_\tau$ denotes the Hilbert transform with respect to τ.

Indeed no other choice for $\mathcal{E}_{ik}(\mathbf{x}_1, \mathbf{x}_2, \tau)$ is really possible since[4]

$$\langle E_i(\mathbf{x}_1, t + \tau)E_k(\mathbf{x}_2, t)\rangle = \langle E_j^*(\mathbf{x}_1, t + \tau)E_k^*(\mathbf{x}_2, t)\rangle = 0. \tag{10}$$

For higher-order moments the choice is not so clearly prescribed. It is shown in Sec. 2 that

$$\langle E_i(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t + \tau_2) \cdots E_p(\mathbf{x}_n, t + \tau_n)\rangle = 0 \qquad n \geq 2, \tag{11}$$

but this still allows a freedom of choice for $n = 3$ and $n = 4$. To remove the remaining ambiguity it will be required that the real part of T_{ikl} or L_{iklm}, the complex representations one associates with T_{ikl}^{rrr} and L_{iklm}^{rrrr}, be equal to a constant times T_{ikl}^{rrr} and L_{iklm}^{rrrr}. The expressions for T_{ikl} and L_{iklm} so obtained will be given in Sec. 3.

In the second-order problem we determine $\mathcal{E}_{ik}(\mathbf{x}_1, \mathbf{x}_2, \tau)$ in the far field as an integral over $\mathcal{E}_{rm}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau_S)$, where the S subscript indicates points on the surface of the source. For $n = 3$ and $n = 4$ no such simple relationship exists. We thus discuss the propagation problem in detail in Sec. 4 to show how the complex formalism may be used. To show how the formalism may be simplified in a particular case we conclude this paper with a disucssion of quasimonochromatic radiation. In particular, in Sec. 6 we treat the problem of determining the two-point intensity coherence for quasimonochromatic radiation from a modulated incoherent source.

Although this paper is written in the language of electromagnetic theory, the results are not restricted to this discipline. The material in Secs. 2 and 3 may be applicable to many fields and the radiation studies may prove useful in the mathematically related field of acoustics.

[4] P. Roman and E. Wolf, Nuovo Cimento 17, 462 (1960).

2. PROOF THAT $\langle E_i(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t + \tau_2) \cdots E_p(\mathbf{x}_n, t + \tau_n)\rangle = 0$

To determine the appropriate forms of T_{ikl} and L_{iklm} it is necessary to first prove that $\langle E_i(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t + \tau_2) \cdots E_p(\mathbf{x}_n, t + \tau_n)\rangle = 0$. To do this we follow a proof given by Roman and Wolf[4] for the second order case.

First note that if $E_i^r(\mathbf{x}, t)$ exists for all time $E_i(\mathbf{x}, t)$ will not exist since the Hilbert transform of $E_i^r(\mathbf{x}, t)$ will not exist. To avoid this difficulty we consider the function

$$\begin{aligned} E_i^r(\mathbf{x}, t, T) &= E_i^r(\mathbf{x}, t), \qquad |t| \leq T, \\ &= 0, \qquad |t| > T. \end{aligned} \tag{12}$$

From $E_i^r(\mathbf{x}, t, T)$ we may form the analytic signal

$$E_i(\mathbf{x}, t, T) = E_i^r(\mathbf{x}, t, T) + iE_i^i(\mathbf{x}, t, T), \tag{13}$$

where $E_i^i(\mathbf{x}, t, T)$ is the Hilbert transform of $E_i^r(\mathbf{x}, t, T)$. In subsequent calculations we let $T \to \infty$. We define the time average of quantities like $E_i(\mathbf{x}, t, T)$ by the integral (see Ref. 3)

$$\lim \frac{1}{2T} \int_{-\infty}^{\infty} (\quad)\, dt.$$

Since $E_i(\mathbf{x}, t, T)$ is an analytic signal we may represent it as an integral over positive frequencies

$$E_i(\mathbf{x}, t, T) = \int_0^\infty \exp(-2\pi i\nu t - 2\pi i\nu\tau)\hat{E}_i(\mathbf{x}, \nu, T)\, d\nu. \tag{14}$$

We now find

$$\begin{aligned} &\langle E_i(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t + \tau_2) \cdots E_p(\mathbf{x}_m, t + \tau_n)\rangle \\ &= \lim_{T\to\infty} \frac{1}{2T} \int_{-\infty}^{\infty} \Bigg[\underbrace{\int_0^\infty \cdots \int_0^\infty}_{\substack{n\text{-fold} \\ \text{integral}}} \\ &\quad \times \exp[-2\pi i(\nu_1 + \nu_2 + \cdots + \nu_n)t] \\ &\quad \times \exp[-2\pi i(\nu_2\tau_2 + \cdots + \nu_n\tau_n)] \\ &\quad \times E_i(\mathbf{x}_1, \nu_1, T)E_k(\mathbf{x}_2, \nu_2, T) \cdots \\ &\quad \times E_p(\mathbf{x}_n, \nu_n, T)\, d\nu_1\, d\nu_2 \cdots d\nu_n \Bigg] dt. \end{aligned} \tag{15}$$

Assuming we may interchange orders of integra-

tion,

$$\langle E_i(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t+\tau_2)\cdots E_p(\mathbf{x}_n, t+\tau_n)\rangle$$
$$= \int_0^\infty \cdots \int_0^\infty \exp\left[-2\pi i(\nu_2\tau_2 + \cdots + \nu_n\tau_n)\right]$$
$$\times \lim_{T\to\infty} \frac{1}{2T}\left[E_i(\mathbf{x}_1, \nu_1, T)E_k(\mathbf{x}_2, \nu_2, T)\cdots E_p(\mathbf{x}_n, \nu_n, T)\right]$$
$$\times \delta(\nu_1 + \nu_2 + \cdots + \nu_n)\, d\nu_1\, d\nu_2 \cdots d\nu_n, \qquad (16)$$

where it may be seen that

$$\delta(\nu_1 + \nu_2 + \cdots + \nu_n) = \int_{-\infty}^{\infty} \exp\left[-2\pi i(\nu_1 + \nu_2 + \cdots + \nu_n)t\right] dt.$$

Now since the integrals over $\nu_1, \nu_2, \cdots, \nu_n$ are only over positive values and the delta function allows a contribution to the integral only when one of the ν_i is negative the right-hand side of Eq. (16) is zero and we have

$$\langle E_i(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t+\tau_2)\cdots E_p(\mathbf{x}_n, t+\tau_n)\rangle = 0. \qquad (17)$$

From Eq. (17) one may show that

$$T^{rrr}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = T^{rii}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) + T^{iri}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) + T^{iir}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3), \qquad (18)$$

$$T^{iii}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = T^{irr}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) + T^{rir}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) + T^{rri}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3), \qquad (19)$$

where, for example,

$$T^{rii}_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) \equiv \langle E^r_j(\mathbf{x}_1, t)E^i_k(\mathbf{x}_2, t+\tau_2)E^i_l(\mathbf{x}_3, t+\tau_3)\rangle.$$

Also

$$L^{rrrr}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = -L^{iiii}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{rrii}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{riri}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{riir}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{irri}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{irir}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{iirr}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4), \qquad (20)$$

$$L^{riii}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = +L^{rirr}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{rrir}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{rrri}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) + L^{irrr}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) - L^{irii}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) - L^{iiri}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) - L^{iiir}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4), \qquad (21)$$

where, for example,

$$L^{riii}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = \langle E^r_j(\mathbf{x}_1, t)E^i_k(\mathbf{x}_2, t+\tau_2)E^i_l(\mathbf{x}_3, t+\tau_3)E^i_m(\mathbf{x}_4, t+\tau_4)\rangle.$$

3. FORM OF $T_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3)$ AND $L_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4)$

In the second-order case we have remarked that the form $\langle E_j(\mathbf{x}_1, t+\tau)E^*_k(\mathbf{x}_2, t)\rangle$ was the only natural complex expression to associate with $\langle E^r_j(\mathbf{x}, t+\tau)E^r_k(\mathbf{x}_2, t)\rangle$. [The expression $\langle E^*_j(\mathbf{x}_1, t+\tau)E_k(\mathbf{x}_2, t)\rangle$ is simply the complex conjugate of $\langle E_j(\mathbf{x}_1, t+\tau)E^*_k(\mathbf{x}_2, t)\rangle$ and introduces nothing new.] For $T^{rrr}_{ijk}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3)$, however, there are three expressions that appear immediately if one wishes an associated complex form. They are

$$T^1_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \langle E^*_j(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t+\tau_2)E_l(\mathbf{x}_3, t+\tau_3)\rangle,$$
$$T^2_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \langle E_j(\mathbf{x}_1, t)E^*_k(\mathbf{x}_2, t+\tau_2)E_l(\mathbf{x}_3, t+\tau_3)\rangle, \qquad (22)$$
$$T^3_{jkl}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \langle E_j(\mathbf{x}_1, t)E_k(\mathbf{x}_2, t+\tau_2)E^*_l(\mathbf{x}_3, t+\tau_3)\rangle,$$

or their complex conjugates.

For these functions one finds from Eqs. (18) and (19) (dropping explicit mention of the arguments for simplicity)

$$T^1_{jkl} = 2[T^{rrr}_{jkl} - T^{rii}_{jkl}] + i2[T^{rir}_{jkl} + T^{rri}_{jkl}],$$
$$T^2_{jkl} = 2[T^{rrr}_{jkl} - T^{iri}_{jkl}] + i2[T^{rri}_{jkl} + T^{irr}_{jkl}], \qquad (23)$$
$$T^3_{jkl} = 2[T^{rrr}_{jkl} - T^{iir}_{jkl}] + i2[T^{rir}_{jkl} + T^{irr}_{jkl}].$$

From Eq. (23) we see that T^1_{jkl} is an analytic signal with respect to the variables τ_2 or τ_3, T^2_{jkl} is an analytic signal with respect to the variable τ_3, and T^3_{jkl} is an analytic signal with respect to τ_2. That is, each function is an analytic signal with respect to those variables for which the complex conjugate was not used.

It is usually desirable that the final result of a mathematical calculation be the real quantity T^{rrr}_{jkl} and thus it is important that the complex form T^1_{jkl} associated with T^{rrr}_{jkl} readily yields T^{rrr}_{jkl}. As we

stated in Sec. 1, we shall use this as a criterion for choosing T_{jkl}. In particular, we require that Re $[T_{jkl}]$ = constant times T^{rrr}_{jkl}.

Imposing the above condition, a satisfactory form for T_{jkl} is

$$T_{jkl} \equiv T^1_{jkl} + T^2_{jkl} + T^3_{jkl}. \tag{24}$$

From Eqs. (18) and (19) we find

$$T_{jkl} = 4T^{rrr}_{jkl} + i4T^{iii}_{jkl}. \tag{25}$$

Unfortunately, Re T_{jkl} and Im T_{jkl} are not now related by a single Hilbert transform relation. However, T^{iii}_{jkl} may be found from T^{rrr}_{jkl} by noting that

$$T^{irr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \frac{1}{\pi} \int \frac{T^{rrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, -s, \tau_3 - \tau_2 - s)\, ds}{s + \tau_2}$$

$$T^{iii}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \frac{1}{\pi^2} \iint \frac{T^{irr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, p_2, p_3)\, dp_2\, dp_3}{(p_2 - \tau_2)(p_3 - \tau_3)}. \tag{26}$$

The fourth-order case proceeds similarly except that now one must consider seven functions

$$\begin{aligned}
L^1_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) &= \langle E_j(\mathbf{x}_1, t) E^*_k(\mathbf{x}_2, t + \tau_2) E^*_l(\mathbf{x}_3, t + \tau_3) E_m(\mathbf{x}_4, t + \tau_4) \rangle, \\
L^2_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) &= \langle E_j(\mathbf{x}_1, t) E^*_k(\mathbf{x}_2, t + \tau_2) E_l(\mathbf{x}_3, t + \tau_3) E^*_m(\mathbf{x}_4, t + \tau_4) \rangle, \\
L^3_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) &= \langle E_j(\mathbf{x}_1, t) E_k(\mathbf{x}_2, t + \tau_2) E^*_l(\mathbf{x}_3, t + \tau_3) E^*_m(\mathbf{x}_4, t + \tau_4) \rangle, \\
L^4_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) &= \langle E^*_j(\mathbf{x}_1, t) E_k(\mathbf{x}_2, t + \tau_2) E_l(\mathbf{x}_3, t + \tau_3) E_m(\mathbf{x}_4, t + \tau_4) \rangle, \\
L^5_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) &= \langle E_j(\mathbf{x}_1, t) E^*_k(\mathbf{x}_2, t + \tau_2) E_l(\mathbf{x}_3, t + \tau_3) E_m(\mathbf{x}_4, t + \tau_4) \rangle, \\
L^6_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) &= \langle E_j(\mathbf{x}_1, t) E_k(\mathbf{x}_2, t + \tau_2) E^*_l(\mathbf{x}_3, t + \tau_3) E_m(\mathbf{x}_4, t + \tau_4) \rangle, \\
L^7_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) &= \langle E_j(\mathbf{x}_1, t) E_k(\mathbf{x}_2, t + \tau_2) E_l(\mathbf{x}_3, t + \tau_3) E^*_m(\mathbf{x}_4, t + \tau_4) \rangle.
\end{aligned} \tag{27}$$

Using Eqs. (20) and (21) one can then find the following relations

$$\begin{aligned}
L^1_{jklm} &= 2[L^{rrii}_{jklm} + L^{riri}_{jklm} + L^{iirr}_{jklm} + L^{irir}_{jklm}] \\
&\quad + i2[-L^{rrir}_{jklm} - L^{rirr}_{jklm} + L^{iiri}_{jklm} + L^{irii}_{jklm}], \\
L^2_{jklm} &= 2[L^{rrii}_{jklm} + L^{riir}_{jklm} + L^{iirr}_{jklm} + L^{irri}_{jklm}] \\
&\quad + i2[-L^{rrri}_{jklm} - L^{rirr}_{jklm} + L^{iiir}_{jklm} + L^{irii}_{jklm}], \\
L^3_{jklm} &= 2[L^{riri}_{jklm} + L^{riir}_{jklm} + L^{irir}_{jklm} + L^{irri}_{jklm}] \\
&\quad + i2[-L^{rrri}_{jklm} - L^{rrir}_{jklm} + L^{iiir}_{jklm} + L^{iiri}_{jklm}], \\
L^4_{jklm} &= 2[L^{rrrr}_{jklm} - L^{rrii}_{jklm} - L^{riri}_{jklm} - L^{riir}_{jklm}] \\
&\quad + i2[-L^{riii}_{jklm} + L^{rirr}_{jklm} + L^{rrir}_{jklm} + L^{rrri}_{jklm}], \\
L^5_{jklm} &= 2[L^{rrrr}_{jklm} - L^{rrii}_{jklm} - L^{iirri}_{jklm} - L^{iirr}_{jklm}] \\
&\quad + i2[-L^{iiri}_{jklm} + L^{irrr}_{jklm} + L^{rrir}_{jklm} + L^{rrri}_{jklm}], \\
L^6_{jklm} &= 2[L^{rrrr}_{jklm} - L^{riri}_{jklm} - L^{iirri}_{jklm} - L^{iirr}_{jklm}] \\
&\quad + i2[-L^{iiri}_{jklm} + L^{irrr}_{jklm} + L^{rirr}_{jklm} + L^{rrri}_{jklm}], \\
L^7_{jklm} &= 2[L^{rrrr}_{jklm} - L^{riir}_{jklm} - L^{irir}_{jklm} - L^{iirr}_{jklm}] \\
&\quad + i2[-L^{iiir}_{jklm} + L^{irrr}_{jklm} + L^{rirr}_{jklm} + L^{rrir}_{jklm}].
\end{aligned} \tag{28}$$

From Eq. (28) we see that L^1_{jklm} is an analytic signal with respect to τ_4; L^2_{jklm} is an analytic signal with respect to τ_3; L^3_{jklm} is an analytic signal with respect to τ_2; L^4_{jklm} is an analytic signal with respect to τ_2, τ_3, or τ_4; L^5_{jklm} is an analytic signal with respect to τ_3 or τ_4; L^6_{jklm} is an analytic signal with respect to τ_2 or τ_4; and L^7_{jklm} is an analytic signal with respect to τ_2 or τ_3.

The function L_{jklm} whose real part is proportional to L^{rrrr}_{jklm} is

$$L_{jklm} = \sum_{p=1}^{7} L^p_{jklm}, \tag{29}$$

where from Eqs. (20) and (21) we find

$$L_{jklm} = 8L^{rrrr}_{jklm} + i4[L^{rirr}_{jklm} + L^{rrir}_{jklm} + L^{rrri}_{jklm} + L^{riii}_{jklm}]. \tag{30}$$

There is no simple relation between Re L_{jklm} and Im L_{jklm} although Im L_{jklm} may be obtained from Re L_{jklm} by noting that all the imaginary terms are simply Hilbert transforms of L^{rrrr}_{jklm}. The relationship between L^{rrrr}_{jklm} and L^{irrr}_{jklm} (which will be needed later) is

$$L^{irrr}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = \frac{1}{\pi} \int \frac{L^{rrrr}_{jklm}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, -s, \tau_3 - \tau_2 - s, \tau_4 - \tau_2 - s)\, ds}{s + \tau_2}.$$

4. SOLUTION OF A RADIATION PROBLEM USING THIRD- AND FOURTH-ORDER MOMENTS

Let us[5] suppose the statistical properties of the radiation field are specified over a finite enclosed surface, S, and we seek the statistical properties of the field external to S. For simplicity we consider the scalar problem (say the forward radiation from a plane finite surface) and replace $E_i^r(\mathbf{x}, t)$ by $V^r(\mathbf{x}, t)$ where $V^r(\mathbf{x}, t)$ satisfies the wave equation

$$\nabla^2 V^r(\mathbf{x}, t) = \frac{1}{c^2}\frac{\partial^2 V^r(\mathbf{x}, t)}{\partial t^2}. \tag{31}$$

We now associate with $V^r(\mathbf{x}, t)$ the truncated function $V^r(\mathbf{x}, t, T)$ and with $V^r(\mathbf{x}, t, T)$ the analytic signal $V(\mathbf{x}, t, T)$ which satisfies the equation[1]

$$\nabla^2 V(\mathbf{x}, t, T) = \frac{1}{c^2}\frac{\partial^2 V(\mathbf{x}, t, T)}{\partial t^2}. \tag{32}$$

In terms of a Green's function, $V(\mathbf{x}, t, T)$ has the formal solution

$$V(\mathbf{x}, t, T) = -\int_0^\infty e^{-2\pi i\nu t}\left[\int_S \frac{\partial G(\mathbf{x}, \mathbf{x}', \nu)}{\partial n_S}\bigg|_{\mathbf{x}'=\mathbf{x}_S} \times \left\{\int_0^\infty e^{2\pi i\nu t'} V(\mathbf{x}_S, t', T)\, dt'\right\} dS\right] d\nu \tag{33}$$

where $G(\mathbf{x}, \mathbf{x}', \nu)$ satisfies the equation

$$\nabla^2 G(\mathbf{x}, \mathbf{x}', \nu) + k^2 G(\mathbf{x}, \mathbf{x}', \nu) = -\delta(\mathbf{x} - \mathbf{x}') \tag{34}$$

($k = 2\pi\nu/c$), the boundary condition $G(\mathbf{x}, \mathbf{x}_S, \nu) = 0$, and the Sommerfeld radiation condition. $\mathbf{x}_S$ indicate points on the surface S.

A. Review of Second-Order Moment Calculations

The second-order mutual coherence function, $\Gamma(\mathbf{x}_1, \mathbf{x}_2, \tau)$ is defined as

$$\Gamma(\mathbf{x}_1, \mathbf{x}_2, \tau) = \lim_{T\to\infty}\frac{1}{2T}\int_{-\infty}^{\infty} V(\mathbf{x}_1, t+\tau, T)V^*(\mathbf{x}_2, t, T)\, dt \tag{35}$$

and formal manipulation (assuming we may interchange the limit and orders of integration) yields

$$\Gamma(\mathbf{x}_1, \mathbf{x}_2, \tau) = \int_0^\infty e^{-2\pi i\nu\tau}\left\{\int_S\int_S K(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \nu) \times \left[\int_{-\infty}^{\infty}\Gamma(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau')e^{2\pi i\nu\tau'}\, d\tau'\right] dS_1\, dS_2\right\} d\nu, \tag{36}$$

where

$$K(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \nu) = \left[\frac{\partial G(\mathbf{x}_1, \mathbf{x}_1', \nu)}{\partial n_{S_1}}\bigg|_{\mathbf{x}_1'=\mathbf{x}_{1S}}\right] \times \left[\frac{\partial G^*(\mathbf{x}_2, \mathbf{x}_2', \nu)}{\partial n_{S_2}}\bigg|_{\mathbf{x}_2'=\mathbf{x}_{2S}}\right].$$

[5] We use the terms "moments" and "coherence functions" interchangeably in this paper.

The function $\hat{\Gamma}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \nu)$, defined as

$$\hat{\Gamma}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \nu) = \int_{-\infty}^{\infty}\Gamma(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau')e^{2\pi i\nu\tau'}\, d\tau', \tag{37}$$

is the mutual power spectrum.

We note $\Gamma(\mathbf{x}_1, \mathbf{x}_2, \tau) = 2\Gamma^{rr}(\mathbf{x}_1, \mathbf{x}_2, \tau) + i2\Gamma^{ir}(\mathbf{x}_1, \mathbf{x}_2, \tau)$ where $\Gamma^{ir}(\mathbf{x}_1, \mathbf{x}_2, \tau)$ is the Hilbert transform of $\Gamma^{rr}(\mathbf{x}_1, \mathbf{x}_2, \tau)$ with respect to τ. $\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau)$ is assumed known and $\Gamma(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau)$ is determined by adding to $2\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau)$, $2i$ times its Hilbert transform with respect to τ.

To calculate $\Gamma(\mathbf{x}_1, \mathbf{x}_2, \tau)$, however, one need not calculate the Hilbert transform of $\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau)$, for only a knowledge of $\hat{\Gamma}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \nu)$ is required. Now

$$\hat{\Gamma}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \nu) = 2\int_{-\infty}^{\infty}\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau')e^{2\pi i\nu\tau'}\, d\tau' + i2\int_{-\infty}^{\infty}\Gamma^{ir}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau')e^{2\pi i\nu\tau'}\, d\tau'. \tag{38}$$

The second term on the right-hand side of Eq. (38) may be written

$$i\int_{-\infty}^{\infty}\Gamma^{ir}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau')e^{2\pi i\nu\tau'}\, d\tau' = i\int_{-\infty}^{\infty}\frac{1}{\pi}\left[\int_{-\infty}^{\infty}\frac{\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, p)}{p-\tau'}\, dp\right]e^{2\pi i\nu\tau'}\, d\tau', \tag{39}$$

using the definition of the Hilbert transform.

Assuming we may interchange orders of integration, this yields

$$i\int_{-\infty}^{\infty}\Gamma^{ir}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau')e^{2\pi i\nu\tau'}\, d\tau' = -i\int_{-\infty}^{\infty}\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, p)\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{e^{2\pi i\nu\tau'}}{(\tau'-p)}\, d\tau'\, dp = \int_{-\infty}^{\infty}\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, p)e^{2\pi i\nu p}\, dp, \tag{40}$$

since

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{e^{2\pi i\nu\tau'}}{\tau'-p}\, d\tau' = ie^{2\pi i\nu p}.$$

Thus

$$\hat{\Gamma}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \nu) = 4\int_{-\infty}^{\infty}\Gamma^{rr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \tau')e^{2\pi i\nu\tau'}\, d\tau'. \tag{41}$$

Equation (36) is particularly useful for considering quasimonochromatic radiation (see Sec. 5 for definition of quasimonochromatic radiation) since the final integral is only over positive frequencies.

B. Third-Order Moment Calculations

Using Eq. (33) one may calculate $T^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3)$ in terms of $T^1(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \tau_{2S}, \tau_{3S})$. We

find

$$T^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \int_0^\infty \int_0^\infty \exp(-2\pi i\nu_2\tau_2 - 2\pi i\nu_3\tau_3)\Big\{\int_S\int_S\int_S K_3^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2+\nu_3, \nu_2, \nu_3)$$
$$\times \Big(\int_{-\infty}^\infty \int_{-\infty}^\infty T^1(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \tau_2', \tau_3') \exp(2\pi i\nu_2\tau_2' + 2\pi i\nu_3\tau_3')\, d\tau_2'\, d\tau_3'\Big)\, dS_1\, dS_2\, dS_3\Big\}\, d\nu_2\, d\nu_3, \quad (42)$$

where

$$K_3^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2+\nu_3, \nu_2, \nu_3)$$
$$= \left[\frac{\partial G^*(\mathbf{x}_1, \mathbf{x}_1', \nu_2+\nu_3)}{\partial n_{S_1}}\bigg|_{\mathbf{x}_1'=\mathbf{x}_{1S}}\right]$$
$$\times \left[\frac{\partial G(\mathbf{x}_2, \mathbf{x}_2', \nu_2)}{\partial n_{S_2}}\bigg|_{\mathbf{x}_2'=\mathbf{x}_{2S}}\right]\left[\frac{\partial G(\mathbf{x}_3, \mathbf{x}_3', \nu_3)}{\partial n_{S_3}}\bigg|_{\mathbf{x}_3'=\mathbf{x}_{3S}}\right].$$

Similar equations may be derived for T^2 and T^3 with functions K_3^2 and K_3^3 defined as above (see Appendix 1 for definitions of K_3^2 and K_3^3).

T is found from the equation

$$T(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3) = \int_0^\infty \int_0^\infty \exp(-2\pi i\nu_2\tau_2 - 2\pi i\nu_3\tau_3)$$
$$\times \int_S\int_S\int_S K_3^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2+\nu_3, \nu_2, \nu_3)$$
$$\times \hat{T}^1(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2, \nu_3)\, dS_1\, dS_2\, dS_3\, d\nu_2\, d\nu_3$$
$$+ \int_0^\infty \int_0^\infty \exp(2\pi i\nu_2\tau_2 - 2\pi i\nu_3\tau_3)$$
$$\times \int_S\int_S\int_S K_3^2(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2+\nu_3, \nu_2, \nu_3)$$
$$\times \hat{T}^2(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, -\nu_2, \nu_3)\, dS_1\, dS_2\, dS_3\, d\nu_2\, d\nu_3$$
$$+ \int_0^\infty \int_0^\infty \exp(-2\pi i\nu_2\tau_2 + 2\pi i\nu_3\tau_3)$$
$$\times \int_S\int_S\int_S K_3^3(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_3, \nu_2, \nu_2, \nu_3)$$
$$\times \hat{T}^3(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2, -\nu_3)\, dS_1\, dS_2\, dS_3\, d\nu_2\, d\nu_3, \quad (43)$$

where, for example,

$$\hat{T}^1(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2, \nu_3)$$
$$= \iint_{-\infty}^{\infty} T^1(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \tau_2', \tau_3')$$
$$\times \exp(2\pi i\nu_2\tau_2' + 2\pi i\nu_3\tau_3')\, d\tau_2'\, d\tau_3'. \quad (44)$$

(In subsequent sections the hook notation will indicate Fourier transforms with respect to the ν variables.)

Unfortunately, we cannot here find a relation of the form

$$T(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3)$$
$$= O(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \tau_2, \tau_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \tau_2', \tau_3')$$
$$\times T(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \tau_2', \tau_3') \quad (45)$$

where O is some linear integral operator.

Referring to Eq. (23) we see that all the terms comprising T^1, T^2, and T^3 may be found from T^{rrr} by taking Hilbert transforms. However, since we only need $\hat{T}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2, \nu_3)$ the calculation simplifies as in the second-order case. (From here on the functional notation of position vectors will be dropped whenever possible.) Calculation shows

$$\hat{T}^1(\nu_2, \nu_3) = 8\hat{T}^{rrr}(\nu_2, \nu_3), \quad (46)$$

$$\hat{T}^2(-\nu_2, \nu_3) = 4\hat{T}^{rrr}(-\nu_2, \nu_3) + i4\hat{T}^{irr}(-\nu_2, \nu_3), \quad (47)$$

$$\hat{T}^3(\nu_2, -\nu_3) = 4\hat{T}^{rrr}(\nu_2, -\nu_3) + i4\hat{T}^{irr}(\nu_2, -\nu_3). \quad (48)$$

$\hat{T}^{rrr}(\nu_2, \nu_3)$ and $\hat{T}^{irr}(\nu_2, \nu_3)$ are not simply related. However, T^{irr} may be found from T^{rrr} by utilizing the following Hilbert transform

$$T^{irr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \tau_2, \tau_3)$$
$$= \frac{1}{\pi} \int \frac{T^{rrr}(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, -p, \tau_3 - \tau_2 - p)}{p + \tau_2}\, dp. \quad (49)$$

C. Fourth-Order Moment Calculations

Proceeding as in the third-order case

$$L^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = \int_0^\infty \int_0^\infty \int_0^\infty \exp(+2\pi i\nu_2\tau_2 + 2\pi i\nu_3\tau_3 - 2\pi i\nu_4\tau_4)$$
$$\times \Big\{\int_S\int_S\int_S\int_S K_4^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, \nu_2+\nu_3-\nu_4, \nu_2, \nu_3, \nu_4)$$
$$\times \hat{L}^1(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, -\nu_2, -\nu_3, \nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\Big\}\, d\nu_2\, d\nu_3\, d\nu_4, \quad (50)$$

where

$$K_4^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, \nu_2 + \nu_3 - \nu_4, \nu_2, \nu_3, \nu_4)$$
$$= \left[\frac{\partial G(\mathbf{x}_1, \mathbf{x}_1', \nu_2 + \nu_3 - \nu_4)}{\partial n_{S_1}}\bigg|_{\mathbf{x}_1' = \mathbf{x}_{1S}}\right] \times \left[\frac{\partial G^*(\mathbf{x}_2, \mathbf{x}_2', \nu_2)}{\partial n_{S_2}}\bigg|_{\mathbf{x}_2' = \mathbf{x}_{2S}}\right]$$
$$\times \left[\frac{\partial G^*(\mathbf{x}_3, \mathbf{x}_3', \nu_3)}{\partial n_{S_3}}\bigg|_{\mathbf{x}_3' = \mathbf{x}_{3S}}\right] \times \left[\frac{\partial G(\mathbf{x}_4, \mathbf{x}_4', \nu_4)}{\partial n_{S_4}}\bigg|_{\mathbf{x}_4' = \mathbf{x}_{4S}}\right].$$

Similar equations may be derived for L^p ($p = 2$, 3, 4, 5, 6, 7) in which the K_4^p are defined similarly to K_4^1. See Appendix 1 for definitions of K_4^p.

Then L becomes

$$L(\tau_2, \tau_3, \tau_4) = \int_0^\infty \int_0^\infty \int_0^\infty \exp\left[2\pi i(\nu_2\tau_2 + \nu_3\tau_3 - \nu_4\tau_4)\right]$$
$$\times \left[\int_S \int_S \int_S \int_S K_4^1(\nu_2 + \nu_3 - \nu_4, \nu_2, \nu_3, \nu_4)\hat{L}^1(-\nu_2, -\nu_3, \nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\right] d\nu_2\, d\nu_3\, d\nu_4$$
$$+ \int_0^\infty \int_0^\infty \int_0^\infty \exp\left[2\pi i(\nu_2\tau_2 - \nu_3\tau_3 + \nu_4\tau_4)\right]$$
$$\times \left[\int_S \int_S \int_S \int_S K_4^2(\nu_2 - \nu_3 + \nu_4, \nu_2, \nu_3, \nu_4)\hat{L}^2(-\nu_2, \nu_3, -\nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\right] d\nu_2\, d\nu_3\, d\nu_4$$
$$+ \int_0^\infty \int_0^\infty \int_0^\infty \exp\left[2\pi i(-\nu_2\tau_2 + \nu_3\tau_3 + \nu_4\tau_4)\right]$$
$$\times \left[\int_S \int_S \int_S \int_S K_4^3(-\nu_2 + \nu_3 + \nu_4, \nu_2, \nu_3, \nu_4)\hat{L}^3(\nu_2, -\nu_3, -\nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\right] d\nu_2\, d\nu_3\, d\nu_4$$
$$+ \int_0^\infty \int_0^\infty \int_0^\infty \exp\left[2\pi i(-\nu_2\tau_2 - \nu_3\tau_3 - \nu_4\tau_4)\right]$$
$$\times \left[\int_S \int_S \int_S \int_S K_4^4(-\nu_2 - \nu_3 - \nu_4, \nu_2, \nu_3, \nu_4)\hat{L}^4(\nu_2, \nu_3, \nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\right] d\nu_2\, d\nu_3\, d\nu_4$$
$$+ \int_0^\infty \int_0^\infty \int_0^\infty \exp\left[2\pi i(+\nu_2\tau_2 - \nu_3\tau_3 - \nu_4\tau_4)\right]$$
$$\times \left[\int_S \int_S \int_S \int_S K_4^5(\nu_2 - \nu_3 - \nu_4, \nu_2, \nu_3, \nu_4)\hat{L}^5(-\nu_2, \nu_3, \nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\right] d\nu_2\, d\nu_3\, d\nu_4$$
$$+ \int_0^\infty \int_0^\infty \int_0^\infty \exp\left[2\pi i(-\nu_2\tau_2 + \nu_3\tau_3 - \nu_4\tau_4)\right]$$
$$\times \left[\int_S \int_S \int_S \int_S K_4^6(-\nu_2 + \nu_3 - \nu_4, \nu_2, \nu_3, \nu_4)\hat{L}^6(\nu_2, -\nu_3, \nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\right] d\nu_2\, d\nu_3\, d\nu_4$$
$$+ \int_0^\infty \int_0^\infty \int_0^\infty \exp\left[2\pi i(-\nu_2\tau_2 - \nu_3\tau_3 + \nu_4\tau_4)\right]$$
$$\times \left[\int_S \int_S \int_S \int_S K_4^7(-\nu_2 - \nu_3 + \nu_4, \nu_2, \nu_3, \nu_4)\hat{L}^7(\nu_2, \nu_3, -\nu_4)\, dS_1\, dS_2\, dS_3\, dS_4\right] d\nu_2\, d\nu_3\, d\nu_4. \quad (51)$$

In analogy to the second- and third-order cases there is a relation between $\hat{L}^p$ and $\hat{L}^{rrrr}$ and $\hat{L}^{irrr}$. The relations are

$$\hat{L}^1(-\nu_2, -\nu_3, \nu_4) = 8\hat{L}^{rrrr}(-\nu_2, -\nu_3, \nu_4) + 8i\hat{L}^{irrr}(-\nu_2, -\nu_3, \nu_4), \quad (52)$$

$$\hat{L}^2(-\nu_2, \nu_3, -\nu_4) = 8\hat{L}^{rrrr}(-\nu_2, \nu_3, -\nu_4) + 8i\hat{L}^{irrr}(-\nu_2, \nu_3, -\nu_4), \quad (53)$$

$$\hat{L}^3(\nu_2, -\nu_3, -\nu_4) = 8\hat{L}^{rrrr}(\nu_2, -\nu_3, -\nu_4) + 8i\hat{L}^{irrr}(\nu_2, -\nu_3, -\nu_4), \quad (54)$$

$$\hat{L}^4(\nu_2, \nu_3, \nu_4) = 16\hat{L}^{rrrr}(\nu_2, \nu_3, \nu_4), \quad (55)$$

$$\hat{L}^5(-\nu_2, \nu_3, \nu_4) = 8\hat{L}^{rrrr}(-\nu_2, \nu_3, \nu_4) + 8i\hat{L}^{irrr}(-\nu_2, \nu_3, \nu_4), \quad (56)$$

$$\hat{L}^6(\nu_2, -\nu_3, \nu_4) = 8\hat{L}^{rrrr}(\nu_2, -\nu_3, \nu_4) + 8i\hat{L}^{irrr}(\nu_2, -\nu_3, \nu_4), \quad (57)$$

$$\hat{L}^7(\nu_2, \nu_3, -\nu_4) = 8\hat{L}^{rrrr}(\nu_2, \nu_3, -\nu_4) + 8i\hat{L}^{irrr}(\nu_2, \nu_3, -\nu_4). \quad (58)$$

The relationship between $L^{rrrr}(\tau_2, \tau_3, \tau_4)$ and $L^{irrr}(\tau_2, \tau_3, \tau_4)$ is

$$L^{irrr}(\tau_2, \tau_3, \tau_4) = \frac{1}{\pi}\int \frac{L^{rrrr}(-p, \tau_3 - \tau_2 - p, \tau_4 - \tau_2 - p)\, dp}{p + \tau_2}. \quad (59)$$

5. QUASIMONOCHROMATIC APPROXIMATION

In the quasimonochromatic approximation we assume that the spectral width of the radiation, $\Delta\nu$, is very small compared to a mean radiation frequency $\bar{\nu}$ (i.e., $\Delta\nu/\bar{\nu} \ll 1$). For the approximation to be useful, however, we introduce the second assumption that radiation path differences Δl and delay times $c\tau$ are much less than $c/\Delta\nu$. As a rough guide we may take path length in the geometric optics sense, but for a more thorough discussion of this assumption we refer the reader to Beran and Parrent.[1]

In the quasimonochromatic approximation we find that $L^m \approx 0$, $m = 4, 5, 6, 7$. In the quasimonochromatic approximation it is convenient to write $V(\mathbf{x}_1, t)$ as

$$V(\mathbf{x}_1, t) = A(\mathbf{x}_1, t) \exp[-i\bar{\omega}t - i\phi(\mathbf{x}_1, t)] \quad (\bar{\omega} = 2\pi\bar{\nu}), \quad (60)$$

where $A(\mathbf{x}_1, t)$ and $\phi(\mathbf{x}_1, t)$ are slowly varying functions of time compared to $e^{-i\bar{\omega}t}$. $L^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4)$ is then for example

$$L^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = \exp[i\bar{\omega}(\tau_2 + \tau_3 - \tau_4)]\langle A(\mathbf{x}_1, t)A(\mathbf{x}_2, t)A(\mathbf{x}_3, t) \times A(\mathbf{x}_4, t) \exp\{i[-\phi(\mathbf{x}_1, t) + \phi(\mathbf{x}_2, t) + \phi(\mathbf{x}_3, t) - \phi(\mathbf{x}_4, t)]\}\rangle, \quad (61)$$

while

$$L^4(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = \exp[-i\bar{\omega}(\tau_2 + \tau_3 + \tau_4)] \times \langle e^{-2i\bar{\omega}t} A(\mathbf{x}_1, t)A(\mathbf{x}_2, t)A(\mathbf{x}_3, t)A(\mathbf{x}_4, t) \times \exp\{i[+\phi(\mathbf{x}_1, t) - \phi(\mathbf{x}_2, t) - \phi(\mathbf{x}_3, t) - \phi(\mathbf{x}_4, t)]\}\rangle. \quad (62)$$

The factor $e^{-2i\bar{\omega}t}$ in the L^4 expression yields $L^4 \ll L^1$ since $A(\mathbf{x}, t)$ and $\phi(\mathbf{x}, t)$ are slowly varying functions of time. Similarly L^5, L^6, and L^7 may be neglected compared to L^1, L^2, and L^3. Thus Eq. (51) contains only three terms.

$L^{rrrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4)$ is of the form

$$L^{rrrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) = \langle A(\mathbf{x}_1, t)A(\mathbf{x}_2, t)A(\mathbf{x}_3, t)A(\mathbf{x}_4, t) \times \{\cos[\bar{\omega}t + \phi(\mathbf{x}_1, t)]\}\{\cos[\bar{\omega}t + \phi(\mathbf{x}_2, t) + \bar{\omega}\tau_2]\} \times \{\cos[\bar{\omega}t + \phi(\mathbf{x}_3, t) + \bar{\omega}\tau_3]\} \times \{\cos[\bar{\omega}t + \phi(\mathbf{x}_4, t) + \bar{\omega}\tau_4]\}\rangle. \quad (63)$$

In time intervals of the order $1/\bar{\omega}$, $A(\mathbf{x}, t)$, and $\phi(\mathbf{x}, t)$ are approximately constant, and direct calculation shows

$$L^{irrr} \approx -L^{riii}, \quad (64)$$

where now

$$L^{rrrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4) \approx \tfrac{1}{8}\langle A_1A_2A_3A_4 \times [\cos(\phi_1 - \phi_2 + \phi_3 - \phi_4 + \bar{\omega}(-\tau_2 + \tau_3 - \tau_4)) + \cos(\phi_1 - \phi_2 - \phi_3 + \phi_4 + \bar{\omega}(-\tau_2 - \tau_3 + \tau_4)) + \cos(\phi_1 + \phi_2 - \phi_3 - \phi_4 + \bar{\omega}(\tau_2 - \tau_3 - \tau_4))]\rangle,$$

$$[A_i \equiv A(\mathbf{x}_i, t),\ \phi_i \equiv \phi(\mathbf{x}_i, t)]$$

and we remember that the A's and ϕ's are functions of time.

Taking the Fourier transform of $L^{irrr}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \tau_2, \tau_3, \tau_4)$ with respect to τ_2, τ_3, and τ_4 it then follows that

$$\hat{L}^{irrr} \approx i^{-1}\hat{L}^{rrrr} \quad (65)$$

and thus for a quasimonochromatic approximation

$$\hat{L}^1(-\nu_2, -\nu_3, \nu_4) \approx 16\hat{L}^{rrrr}(-\nu_2, -\nu_3, \nu_4), \quad (66)$$

$$\hat{L}^2(-\nu_2, \nu_3, -\nu_4) \approx 16\hat{L}^{rrrr}(-\nu_2, \nu_3, -\nu_4), \quad (67)$$

$$\hat{L}^3(\nu_2, -\nu_3, -\nu_4) \approx 16\hat{L}^{rrrr}(\nu_2, -\nu_3, -\nu_4), \quad (68)$$

$$\hat{L}^4 \approx \hat{L}^5 \approx \hat{L}^6 \approx \hat{L}^7 \approx 0. \quad (69)$$

Finally note that

$$\hat{L}^1(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, -\nu_2, -\nu_3, \nu_4) \approx \langle A_{1S}A_{2S}A_{3S}A_{4S} \exp[i(-\phi_{1S} + \phi_{2S} + \phi_{3S} - \phi_{4S})]\rangle \times \delta(\nu_2 - \bar{\nu})\delta(\nu_3 - \bar{\nu})\delta(\nu_4 - \bar{\nu}) \quad (70)$$

$$\hat{L}^2(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, -\nu_2, \nu_3, -\nu_4) \approx \langle A_{1S}A_{2S}A_{3S}A_{4S} \exp[i(-\phi_{1S} + \phi_{2S} - \phi_{3S} + \phi_{4S})]\rangle \times \delta(\nu_2 - \bar{\nu})\delta(\nu_3 - \bar{\nu})\delta(\nu_4 - \bar{\nu}), \quad (71)$$

$$\hat{L}^3(\mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, \nu_2, -\nu_3, -\nu_4)$$
$$\approx \langle A_{1S}A_{2S}A_{3S}A_{4S} \exp[i(-\phi_{1S} - \phi_{2S} + \phi_{3S} + \phi_{4S})]\rangle$$
$$\times \delta(\nu_2 - \bar{\nu})\delta(\nu_3 - \bar{\nu})\delta(\nu_4 - \bar{\nu}), \quad (72)$$

so that

$$L(0, 0, 0) \approx \int_S \int_S \int_S \int_S K_4^1(\bar{\nu}, \bar{\nu}, \bar{\nu}, \bar{\nu})$$
$$\times \langle V_{1S}V_{2S}^*V_{3S}^*V_{4S}\rangle \, dS_1 \, dS_2 \, dS_3 \, dS_4$$
$$+ \int_S \int_S \int_S \int_S K_4^2(\bar{\nu}, \bar{\nu}, \bar{\nu}, \bar{\nu})$$
$$\times \langle V_{1S}V_{2S}^*V_{3S}V_{4S}^*\rangle \, dS_1 \, dS_2 \, dS_3 \, dS_4$$
$$+ \int_S \int_S \int_S \int_S K_4^3(\bar{\nu}, \bar{\nu}, \bar{\nu}, \bar{\nu})$$
$$\times \langle V_{1S}V_{2S}V_{3S}^*V_{4S}^*\rangle \, dS_1 \, dS_2 \, dS_3 \, dS_4, \quad (73)$$

where

$$V_{iS} = V(\mathbf{x}_{iS}, t) = A(\mathbf{x}_{iS}, t) \exp[-i\phi(\mathbf{x}_{iS}, t)],$$

and we have set $\tau_2 = \tau_3 = \tau_4 = 0$ since in the quasimonochromatic approximation the τ term contributes only an oscillatory factor of no importance.

It is important to realize that the above forms of $\hat{L}^1$, $\hat{L}^2$, and $\hat{L}^3$ may be introduced into Eq. (51) only if the assumption of small path differences and small time delays is valid.

6. QUASIMONOCHROMATIC RADIATION FROM A MODULATED INCOHERENT SOURCE

In this section we consider the problem of dedetermining the two-point intensity coherence function for quasimonochromatic radiation from a modulated incoherent source. This problem was treated by Beran and Parrent[6] in a verbal presentation and we present a similar development here as an illustration of the formalism we have developed. The point of the verbal presentation was to show that it was possible in principle to detect large scale turbulent fluctuations occurring in nonresolvable objects.

By the two-point intensity coherence function we may mean either

$$L^{rrrr}(\mathbf{x}_1, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_3, 0, 0, 0) \equiv R^{rr}(\mathbf{x}_1, \mathbf{x}_3, 0)$$
$$\text{or} \quad L^1(\mathbf{x}_1, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_3, 0, 0, 0) \equiv R^1(\mathbf{x}_1, \mathbf{x}_3, 0).$$

The first function assumes that prior to time averaging, $(V_1^r)^2$ measurements may be made in times of the order of $1/\bar{\nu}$; the second form assumes $(V_1^r)^2$ is averaged over several cycles of the mean wavelength before detection and subsequent time averaging. For our discussion we shall assume some local averaging occurs prior to detection and thus shall calculate $R^1(\mathbf{x}_1, \mathbf{x}_3, 0) = \langle (V_1V_1^*)(V_3V_3^*)\rangle$.

$R^1(\mathbf{x}_1, \mathbf{x}_3, 0)$ is given by the equation [we now need only the first term in Eq. (73)]

$$R^1(\mathbf{x}_1, \mathbf{x}_3, 0) = \int_S \int_S \int_S \int_S K_4^1(\bar{\nu}, \bar{\nu}, \bar{\nu}, \bar{\nu})$$
$$\times \langle V_{1S}V_{2S}^*V_{3S}^*V_{4S}\rangle \, dS_1 \, dS_2 \, dS_3 \, dS_4. \quad (74)$$

We wish to calculate $R^1(\mathbf{x}_1, \mathbf{x}_3, 0)$ for quasimonochromatic radiation from a modulated incoherent source. We first consider the calculation for an unmodulated incoherent source. For an incoherent source we will assume here that the statistics are Gaussian, that the phase and amplitude at a point at uncorrelated, and that the phase has equal probability of being anywhere between 0 and 2π. (An incoherent source has never been properly defined and so these assumptions may in a sense be taken to be part of our definition of an incoherent source. Note, however, that we here consider only quasimonochromatic radiation from an incoherent source since otherwise the concepts of phase and amplitude would be meaningless. Basically we have in mind radiation similar to filtered starlight.) Thus,

$$\langle V_{1S}V_{2S}^*V_{3S}^*V_{4S}\rangle = \langle V_{1S}V_{2S}^*\rangle\langle V_{3S}^*V_{4S}\rangle$$
$$+ \langle V_{1S}V_{3S}^*\rangle\langle V_{2S}^*V_{4S}\rangle. \quad (75)$$

Equation (A4) gives the form of K_4^1 and thus we have finally

$$R^1(\mathbf{x}_1, \mathbf{x}_3, 0) = \left[\int_S \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_1, \mathbf{x}_{2S}, \bar{\nu})\langle V_{1S}V_{2S}^*\rangle \, dS_1 \, dS_2\right]$$
$$\times \left[\int_S \int_S H^*(\mathbf{x}_3, \mathbf{x}_{3S}, \bar{\nu})H(\mathbf{x}_3, \mathbf{x}_{4S}, \bar{\nu})\langle V_{3S}^*V_{4S}\rangle \, dS_3 \, dS_4\right]$$
$$+ \left[\int_S \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_3, \mathbf{x}_{3S}, \bar{\nu})\langle V_{1S}V_{3S}^*\rangle \, dS_1 \, dS_3\right]$$
$$\times \left[\int_S \int_S H^*(\mathbf{x}_1, \mathbf{x}_{2S}, \bar{\nu})H(\mathbf{x}_3, \mathbf{x}_{4S}, \bar{\nu})\langle V_{2S}^*V_{4S}\rangle \, dS_2 \, dS_4\right], \quad (76)$$

[6] M. Beran and G. B. Parrent, Jr., J. Opt. Soc. Am. 52, 98 (1961).

$$R^1(\mathbf{x}_1, \mathbf{x}_3, 0) = \hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_1, \bar{\nu})\hat{\Gamma}(\mathbf{x}_3, \mathbf{x}_3, \bar{\nu}) + \hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_3, \bar{\nu})\hat{\Gamma}^*(\mathbf{x}_1, \mathbf{x}_3, \bar{\nu}), \quad (77)$$

$$R^1(\mathbf{x}_1, \mathbf{x}_3, 0) = \hat{I}(\mathbf{x}_1, \bar{\nu})\hat{I}(\mathbf{x}_3, \bar{\nu}) + |\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_3, \bar{\nu})|^2. \quad (78)$$

Here

$$\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_3, \bar{\nu}) = \int_S \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_3, \mathbf{x}_{3S}, \bar{\nu})\langle V_{1S}V_{3S}^*\rangle \, dS_1 \, dS_3$$

$$\hat{I}(\mathbf{x}_1, \bar{\nu}) = \hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_1, \bar{\nu}).$$

Since we are dealing with an incoherent source the expression for $\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_3, \bar{\nu})$ could be simplified. Beran and Parrent[7] have shown that for radiation in the far field, when a scalar theory is applicable $\langle V_{1S}V_{3S}^*\rangle$ may be replaced by $\beta\langle V_{1S}V_{1S}^*\rangle \, \delta(S_1 - S_3)$, where β is a constant that depends upon the frequency and details of the source. Then

$$\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_3, \bar{\nu}) = \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_3, \mathbf{x}_{1S}, \bar{\nu}) \times \beta\langle V_{1S}V_{1S}^*\rangle \, dS_1. \quad (79)$$

Lastly, assuming the intensity is constant over the source surface, we have

$$\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_3, \bar{\nu}) = \alpha \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_3, \mathbf{x}_{1S}, \bar{\nu}) \, dS_1, \quad (80)$$

where α is a constant. This yields

$$R^1(\mathbf{x}_1, \mathbf{x}_3, 0) = \hat{I}(\mathbf{x}_1, \bar{\nu})\hat{I}(\mathbf{x}_3, \bar{\nu}) + \alpha^2 \left| \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_3, \mathbf{x}_{1S}, \bar{\nu}) \, dS_1 \right|^2. \quad (81)$$

By a modulated incoherent source we mean here a source that undergoes intensity variations with period $\tau_T \ll 1/\Delta\nu$. This is the effect turbulent fluctuations would have on the radiation passing through a surface immediately surrounding an incoherent source. To distinguish the slow intensity fluctuations from the rapid fluctuations of order $1/\Delta\nu$ we introduce the concept on an ensemble of time intervals. We assume that $\langle V_{1S}V_{2S}^*V_{3S}^*V_{4S}\rangle$ has the form

$$\langle V_{1S}V_{2S}^*V_{3S}^*V_{4S}\rangle = \langle V_{1S}V_{2S}^*\rangle_n\langle V_{3S}^*V_{4S}\rangle_n + \langle V_{1S}V_{3S}^*\rangle_n\langle V_{2S}^*V_{4S}\rangle_n \quad (82)$$

in each of a series of $n = 1, 2, \cdots, N$ time intervals of length τ_E, where $1/\Delta\nu \ll \tau_E \ll \tau_T$. $\langle \ \rangle_n$ now indicates a time average over a time τ_E in the nth interval. It is assumed that in each interval the intensity at points on S are essentially constant, but that the intensity may change from interval to interval. To find the average effects of the intensity fluctuations we simply average over the ensemble of time intervals. We denote this averaging by boldface square brackets, $[\ ]_{\mathrm{av}}$. In other words we now compute

$$[R_n^1(\mathbf{x}_1, \mathbf{x}_3, 0)]_{\mathrm{av}} = \int_S \int_S \int_S \int_S K_4^1(\bar{\nu}, \bar{\nu}, \bar{\nu})\{[\langle V_{1S}V_{2S}^*\rangle_n\langle V_{3S}^*V_{4S}\rangle_n]]_{\mathrm{av}} + [[\langle V_{1S}V_{3S}^*\rangle_n\langle V_{2S}^*V_{4S}\rangle_n]]_{\mathrm{av}}\} \, dS_1 \, dS_2 \, dS_3 \, dS_4. \quad (83)$$

For an incoherent source we have

$$\langle V_{iS}V_{jS}^*\rangle_n = \beta I_{iSn}(\mathbf{x}_{iS})\delta(S_i - S_j). \quad (84)$$

Therefore, Eq. (84) yields

$$\langle R_n^1(\mathbf{x}_1, \mathbf{x}_3, 0)\rangle = \beta^2 \int_S \int_S |H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})|^2 \, |H(\mathbf{x}_3, \mathbf{x}_{3S}, \bar{\nu})|^2 \times [I_{1Sn}(\mathbf{x}_{1S})I_{3Sn}(\mathbf{x}_{3S})]_{\mathrm{av}} \, dS_1 \, dS_3 + \beta^2 \int_S \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_3, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_1, \mathbf{x}_{2S}, \bar{\nu}) \times H(\mathbf{x}_3, \mathbf{x}_{2S}, \bar{\nu})[I_{1Sn}(\mathbf{x}_{1S})I_{2Sn}(\mathbf{x}_{2S})]_{\mathrm{av}} \, dS_1 \, dS_2. \quad (85)$$

If we now write

$$I_{jSn}(\mathbf{x}_{jS}) = [I_{jS}(\mathbf{x}_{jS})]_{\mathrm{av}} + I'_{jSn}(\mathbf{x}_{jS})$$

then

$$[R_n^1(\mathbf{x}_1, \mathbf{x}_3, 0)]_{\mathrm{av}} = R_0^1(\mathbf{x}_1, \mathbf{x}_3, 0) + \beta^2 \int_S \int_S |H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})|^2 \, |H(\mathbf{x}_3, \mathbf{x}_{3S}, \bar{\nu})|^2 \times [I'_{1Sn}(\mathbf{x}_{1S})I'_{3Sn}(\mathbf{x}_{3S})]_{\mathrm{av}} \, dS_1 \, dS_3 + \beta^2 \int_S \int_S H(\mathbf{x}_1, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_3, \mathbf{x}_{1S}, \bar{\nu})H^*(\mathbf{x}_1, \mathbf{x}_{2S}, \bar{\nu}) \times H(\mathbf{x}_3, \mathbf{x}_{2S}, \bar{\nu})[I'_{1Sn}(\mathbf{x}_{1S})I'_{2Sn}(\mathbf{x}_{2S})]_{\mathrm{av}} \, dS_1 \, dS_2, \quad (86)$$

where $R_0^1(\mathbf{x}_1, \mathbf{x}_3, 0)$ is the solution in the absence of modulation.

To proceed further we suppose the source surface is plane and that

$$[I'_{jSn}(\mathbf{x}_{jS})I'_{kSn}(\mathbf{x}_{kS})]_{\mathrm{av}} = \sigma(|\mathbf{x}_{jS} - \mathbf{x}_{kS}|).$$

[7] M. Beran and G. B. Parrent, Jr., Nuovo Cimento 27, 1049 (1963).

For a plane surface $H(\mathbf{x}_i, \mathbf{x}_{kS}, \bar{\nu})$ is (see Beran and Parrent[1])

$$H(\mathbf{x}_i, \mathbf{x}_{kS}, \bar{\nu}) = \frac{-2(1 - ikr_{ikS})}{4\pi} \frac{z_i}{(r_{ikS})^3} \exp(ikr_{ikS}), \tag{87}$$

where

$$r_{ikS} = ((x_i - x_{kS})^2 + (y_i - y_{kS})^2 + (z_i - z_{kS})^2)^{\frac{1}{2}}.$$

In the forward region of the far field of the source this expression simplifies to

$$H(\mathbf{x}_i, \mathbf{x}_{kS}, \bar{\nu}) = \frac{ik}{2\pi R} \exp\left[-\frac{ik}{R}(x_{kS}x_i + y_{kS}y_i)\right] e^{ikR}, \tag{88}$$

where R is the distance from some point on the source surface to the observation point. Substituting Eq. (88) into Eq. (86) yields

$$[R_n^1(\mathbf{x}_1, \mathbf{x}_3, 0)]_{av} = R_0^1(\mathbf{x}_1, \mathbf{x}_3, 0) + \frac{\beta^2 k^4}{16\pi^4 R^4}\left(\int_S\int_S \sigma(|\mathbf{x}_{1S} - \mathbf{x}_{3S}|)\, dS_1\, dS_3 + \int_S\int_S \sigma(|\mathbf{x}_{1S} - \mathbf{x}_{2S}|)\right.$$
$$\left. \times \exp\left[-\frac{ik}{R}(x_{1S}x_1 + y_{1S}y_1 - x_{1S}x_3 - y_{1S}y_3)\right] \exp\left[-\frac{ik}{R}(-x_{2S}x_1 - y_{2S}y_1 + x_{2S}x_3 + y_{2S}y_3)\right] dS_1\, dS_2\right). \tag{89}$$

Changing to the coordinates $\mathbf{x}_{12} = \mathbf{x}_{1S} - \mathbf{x}_{2S}$, $\mathbf{x}'_{1S} = \mathbf{x}_{1S}$, we have

$$[R_n^1(\mathbf{x}_1, \mathbf{x}_3, 0)]_{av} = R_0^1(\mathbf{x}_1, \mathbf{x}_3, 0) + \frac{\beta^2 k^4}{16\pi^4 R^4}\left\{\int_S\left[\int_0^\infty\int_0^{2\pi} \sigma(r_{12}) r_{12}\, dr_{12}\, d\theta\right] dS'_1\right.$$
$$\left. + \int_S\left(\iint_{-\infty}^{\infty} \sigma(r_{12}) \exp\left[-\frac{ik}{R}[(x_1 - x_3)x_{12} + (y_1 - y_3)y_{12}]\right] dx_{12}\, dy_{12}\right) dS'_1\right\} \tag{90}$$

assuming $\sigma(r_{12}) \to 0$ in distances small compared to a characteristic dimension of the source area. This yields

$$[R_n^1(\mathbf{x}_1, \mathbf{x}_3, 0)]_{av} = R_0^1(\mathbf{x}_1, \mathbf{x}_3, 0)$$
$$+ \frac{\beta^2 k^4}{16\pi^4 R^4} A\left[2\pi[(I')^2]_{av} l^2 + 2\pi \int_0^\infty \sigma(r_{12}) r_{12} J_0\left(((x_1 - x_3)^2 + (y_1 - y_3)^2)^{\frac{1}{2}} \frac{k}{R} r_{12}\right)\right] dr_{12}, \tag{91}$$

where $[(I')^2]_{av} l^2 = \int_0^\infty r_{12}\sigma(r_{12})\, dr_{12}$.

When $\mathbf{x}_1 = \mathbf{x}_3$ we find

$$\frac{2\pi[(I')^2]_{av} l^2 A\beta^2 k^4}{16\pi^4 R^4} = [R_n^1(\mathbf{x}_1, \mathbf{x}_1, 0)]_{av} - R_0^1(\mathbf{x}_1, \mathbf{x}_1, 0), \tag{92}$$

thus $[(I')^2]_{av} l^2$ is measurable if we measure $[R_n^1(\mathbf{x}_1, \mathbf{x}_1, 0)]_{av}$ and $\Gamma(\mathbf{x}_1, \mathbf{x}_1, 0)$ [Note that $\Gamma(\mathbf{x}_1, \mathbf{x}_1, 0)$ is insensitive to the modulation.] and calculate $R_0^1(\mathbf{x}_1, \mathbf{x}_1, 0)$ from $\Gamma(\mathbf{x}_1, \mathbf{x}_1, 0)$. The function

$$P(\mathbf{x}_1, \mathbf{x}_3, 0) = \frac{16\pi^4 R^4}{2\pi\beta^2 k^4 A}[[R_n^1(\mathbf{x}_1, \mathbf{x}_3, 0)]_{av}$$
$$- R_0^1(\mathbf{x}_1, \mathbf{x}_3, 0)] - l^2[(I')^2]_{av} \tag{93}$$

may similarly be determined by measurement and calculation. We have then (setting $x_1 = y_1 = 0$ for convenience)

$$\int_0^\infty \sigma(r_{12}) r_{12}\, dr_{12} J_0\left(d\frac{k}{R} r_{12}\right) = P(d, 0), \tag{94}$$

where $d = (x_3^2 + y_3^2)^{\frac{1}{2}}$. $P(d, 0)$ is the Bessel transform of $\sigma(r_{12})$ and the integral may be inverted to yield $\sigma(r_{12})$.

At the origin the ratio of $R_0^1(\mathbf{x}_1, \mathbf{x}_1, 0)$ to

$$\frac{\beta^2 k^4}{16\pi^4 R^4} A 2\pi[(I')^2]_{av} l^2$$

is $\approx D^2\bar{I}^2/l^2[(I')^2]_{av}$, where D is a characteristic source dimension. Interpreting $[(I')^2]_{av}$ as the mean square fluctuation in intensity, l is a macroscale of the modulation. The characteristic spread of $R^1(\mathbf{x}_1, \mathbf{x}_3, 0)$ is R/kD, and the characteristic spread of the integral in Eq. (92) is R/kl.

To detect the modulation is extremely difficult unless l is a significant fraction of D and the intensity fluctuations are appreciable. The fact that $R/kD \ll R/kl$ is an aid in detection however, since the modulation effect becomes a much more significant fraction of the unmodulated effect when $|\mathbf{x}_1 - \mathbf{x}_3| \gg R/kD$.

APPENDIX I

$$K_3^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2 + \nu_3, \nu_2, \nu_3) = H^*(\mathbf{x}_1, \mathbf{x}_{1S}, \nu_2 + \nu_3)H(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3), \tag{A1}$$

where

$$H(\mathbf{x}_p, \mathbf{x}_{pS}, \nu) = \frac{\partial G(\mathbf{x}_p, \mathbf{x}_p', \nu)}{\partial n_{S_p}}\bigg|_{\mathbf{x}_p' = \mathbf{x}_{pS}}.$$

$$K_3^2(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_2 - \nu_3, \nu_2, \nu_3) = H(\mathbf{x}_1, \mathbf{x}_{1S}, \nu_2 - \nu_3)H^*(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3). \tag{A2}$$

$$K_3^3(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \nu_3 - \nu_2, \nu_2, \nu_3) = H(\mathbf{x}_1, \mathbf{x}_{1S}, \nu_3 - \nu_2)H(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H^*(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3). \tag{A3}$$

$$K_4^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, \nu_2 + \nu_3 - \nu_4, \nu_3, \nu_4)$$
$$= H(\mathbf{x}_1, \mathbf{x}_{1S}, \nu_2 + \nu_3 - \nu_4)H^*(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H^*(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3)H(\mathbf{x}_4, \mathbf{x}_{4S}, \nu_4). \tag{A4}$$

$$K_4^2(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, \nu_2 - \nu_3 + \nu_4, \nu_3, \nu_4)$$
$$= H(\mathbf{x}_1, \mathbf{x}_{1S}, \nu_2 - \nu_3 + \nu_4)H^*(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3)H^*(\mathbf{x}_4, \mathbf{x}_{4S}, \nu_4). \tag{A5}$$

$$K_4^3(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, -\nu_2 + \nu_3 + \nu_4, \nu_3, \nu_4)$$
$$= H(\mathbf{x}_1, \mathbf{x}_{1S}, -\nu_2 + \nu_3 + \nu_4)H(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H^*(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3)H^*(\mathbf{x}_4, \mathbf{x}_{4S}, \nu_4). \tag{A6}$$

$$K_4^4(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, \nu_2 + \nu_3 + \nu_4, \nu_2, \nu_3, \nu_4)$$
$$= H^*(\mathbf{x}_1, \mathbf{x}_{1S}, \nu_2 + \nu_3 + \nu_4)H(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3)H(\mathbf{x}_4, \mathbf{x}_{4S}, \nu_4). \tag{A7}$$

$$K_4^5(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_4, \nu_2 - \nu_3 - \nu_4, \nu_2, \nu_3, \nu_4)$$
$$= H(\mathbf{x}_1, \mathbf{x}_{1S}, \nu_2 - \nu_3 - \nu_4)H^*(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3)H(\mathbf{x}_4, \mathbf{x}_{4S}, \nu_4). \tag{A8}$$

$$K_4^6(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, -\nu_2 + \nu_3 - \nu_4, \nu_2, \nu_3, \nu_4)$$
$$= H(\mathbf{x}_1, \mathbf{x}_{1S}, -\nu_2 + \nu_3 - \nu_4)H(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H^*(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3)H(\mathbf{x}_4, \mathbf{x}_{4S}, \nu_4). \tag{A9}$$

$$K_4^7(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_{1S}, \mathbf{x}_{2S}, \mathbf{x}_{3S}, \mathbf{x}_{4S}, -\nu_2 - \nu_3 + \nu_4, \nu_2, \nu_3, \nu_4)$$
$$= H(\mathbf{x}_1, \mathbf{x}_{1S}, -\nu_2 - \nu_3 + \nu_4)H(\mathbf{x}_2, \mathbf{x}_{2S}, \nu_2)H(\mathbf{x}_3, \mathbf{x}_{3S}, \nu_3)H^*(\mathbf{x}_4, \mathbf{x}_{4S}, \nu_4). \tag{A10}$$

Derivation of Low-Temperature Expansions for the Ising Model of a Ferromagnet and an Antiferromagnet

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Low-temperature expansions for the free energy of the Ising model of a ferromagnet and an antiferromagnet are derived for the more usual two- and three-dimensional lattices. The underlying enumerative problem is studied and a new method described that makes it possible to obtain more terms than available previously without undue labor.

1. INTRODUCTION

THE theory of cooperative phenomena in crystals has received much attention in recent years and considerable effort has been given to the elucidation of the properties of the three-dimensional Ising model. For a general introduction and a lead into the literature reference should be made to the review by Domb[1] and more recently by Fisher.[2]

One of the most successful methods so far employed in investigations of the physical properties of the Ising model, be it for a ferromagnet, antiferromagnet, binary alloy, or lattice gas, is a study of exact series expansions. By a study of these the problem of the critical behavior of the spontaneous magnetization, specific heat, and susceptibility, for the three-dimensional model has been largely resolved.[3-5] Extrapolation procedures have been much improved recently[5] and it is becoming clear that the method can yield useful information if expansions of adequate length are available.

It is the purpose of this paper to investigate the enumerative problem that arises in the derivation of what are usually described as "low-temperature" expansions. We shall describe a new method and use it to derive data sufficient for most applications for the more usual two- and three-dimensional lattices. In most cases our results represent a useful advance on the data available hitherto. The new method exploits the well-known sublattice division of loose-packed lattices and is especially effective for the derivation of expansions for the antiferrimagnetic problem. It has a further advantage, of great practical value, of being to a large extent self-checking. It is, therefore, possible to undertake with confidence complex enumerations that would be otherwise difficult to verify.

The data have already been applied in part to the ferromagnetic problem,[6,7] antiferromagnetic problem,[8-10] and the binary alloy problem.[11] The retention of the sublattice division allows one to study the Ising antiferromagnet in a magnetic field while retaining a parameter (the staggered field susceptibility) which should have a strong singularity at the critical temperature.

The method described can be modified for a study of more complex systems such as, for example, ferrimagnetism or the nonstoichiometric alloy problem with nearest-neighbor interactions, which, if we neglect the change of thermal vibrations with ordering, is formally equivalent to the Ising model in a temperature-dependent magnetic field. We give in the text an account of some applications and an assessment of the data derived.

2. THE LOW-TEMPERATURE ENUMERATIVE PROBLEM FOR A FERROMAGNET

The low-temperature enumerative problem arises quite naturally in the derivation of low-temperature

[1] C. Domb, Advan. Phys. 9, Nos. 34 and 35 (1960).
[2] M. E. Fisher, J. Math. Phys. 4, 278 (1963).
[3] C. Domb and M. F. Sykes, J. Math. Phys. 2, 63 (1963).
[4] G. A. Baker, Phys. Rev. 129, 99 (1963).
[5] G. A. Baker, Phys. Rev. 124, 768 (1961).
[6] J. W. Essam and M. E. Fisher, J. Chem. Phys. 38, 802 (1963).
[7] M. E. Fisher (to be published).
[8] M. F. Sykes and M. E. Fisher, Physica 28, 919 (1962).
[9] M. E. Fisher and M. F. Sykes, Physica 28, 939 (1962).
[10] J. W. Essam and M. F. Sykes, Physica 29, 378 (1963).
[11] A. Bienenstock (to be published).

expansions for the free energy of the Ising model. At absolute zero all the spins point one way and give rise to a spontaneous magnetization, and for temperatures slightly above zero thermal fluctuations will perturb this ordered state. The probability of any particular perturbation will be given by the appropriate Boltzmann factor and, in general, the overturning of a spin causes an increase in energy. The most important perturbations at the lowest temperatures will thus correspond to relatively few overturned spins. The possible perturbations are conveniently grouped by the number of overturned spins and the energy of any particular perturbation depends on the relative positions of these overturned spins. If, following the usual convention, we denote by $2J$ the energy gained if two first-neighbor spins change from parallel to antiparallel position, and denote by m the magnetic moment per spin, it is readily shown that the overturning of s spins with r first-neighbor bonds between them results in an energy gain of

$$2(qs - 2r)J + 2msH, \tag{2.1}$$

where H denotes any applied magnetic field and q is the coordination number. Denoting

$$\exp(-4J/kT) \text{ by } u = z^2 \text{ and } \exp(-2mH/kT) \text{ by } \mu, \tag{2.2}$$

the Boltzmann factor corresponding to (2.1) will be

$$\exp\{[-2(qs - 2r)J - 2msH]/kT\} = u^{\frac{1}{2}qs-r}\mu^s \tag{2.3}$$

and the energy of the ground state is

$$-N(\tfrac{1}{2}qJ + mH). \tag{2.4}$$

At low temperatures both u and μ are small and the partition function and free energy can be expanded as a double series in powers of u and μ. Following the notation of Domb we shall write the free energy per spin (F) as

$$F = -\tfrac{1}{2}qJ - mH - kT \ln \Lambda(\mu, u). \tag{2.5}$$

To derive the series development for $\ln \Lambda$ we must study perturbations of the ordered state.

In general, the number of perturbations of a given type on an infinite lattice of N sites will be some polynomial in N and it can be shown that the contribution to the configurational free energy per spin corresponds to taking the coefficient of the first power of N. Denoting this linear part of the total number of ways of choosing s spins with r bonds between them by $[s; r]$ then

$$\ln \Lambda = \sum_{\text{all } s,r} [s; r]u^{\frac{1}{2}qs-r}\mu^s. \tag{2.6}$$

We shall group the expansion (2.6) as a development in powers of μ and the successive coefficients will then be finite polynomials in u, $L_s(u)$ defined by

$$\ln \Lambda = \sum_s L_s(u)\mu^s. \tag{2.7}$$

To specify a polynomial L_s we require the contributions from perturbations with s overturned spins.

$$L_s(u) = \sum_{r=0}^{\frac{1}{2}s(s-1)} [s; r]u^{\frac{1}{2}qs-r}. \tag{2.8}$$

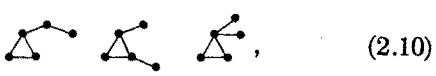
The most complete description of the various perturbations that make up any given $[s; r]$ is provided by grouping them according to the topology of their nearest-neighbor linkages. We may call this the *method of topological breakdown*. As an example on the face-centered cubic lattice the perturbations corresponding to [4; 3] are, in a self-explanatory notation,

(1)  $(282N)$

(2)  $(44N)$ Total contribution to [4; 3] = 126. (2.9)

(3)  $(8N^2 - 200N)$

Methods for counting such low-temperature configurations, as these are called, have been much studied by Domb[1] and his co-workers. For all but the smallest values of s it is convenient to count the terms in a contracted notation. For example, in [5; 5] we require the values of perturbations corresponding to the configurations

 (2.10)

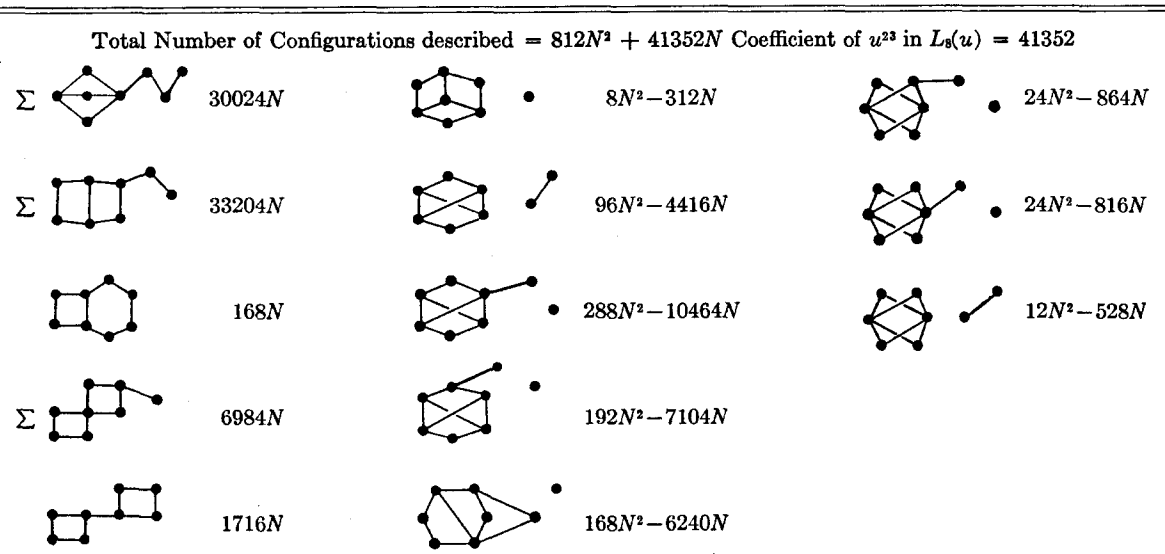
and we shall denote the total contribution of these by

Σ  . (2.11)

With this convention we illustrate in Fig. 1 the topological breakdown of [8; 9] on the body-centered cubic lattice. It is evident that descriptions of this kind are laborious to derive. We shall obtain the result [8; 9] = 41352 on the body-centered cubic more directly in Sec. 4.

We give in Appendix I a table of the perturbations of up to 5 spins for the triangular and face-centered cubic lattices. To derive a useful number of terms it is usual to exploit the fact that the $\frac{1}{2}s(s-1)+1$ quantities $[s; 0]$, $[s; 1]$, $\cdots$, $[s; \frac{1}{2}s(s-1)]$ are not all independent and it is possible to derive s linear relations between them. These constraints

FIG. 1. Body-centered cubic—synoptic topological breakdown for [8; 9].



have been described by Domb[12] and applied to the simple quadratic lattice. A further application was made by Wakefield[13] to the simple cubic lattice. A proof of these constraints for the simple cubic lattice which holds without modification for any loose-packed lattice has been given by Wakefield and the result for close-packed lattices has been proved by Sykes.[14] The generalization of these constraints to the second-neighbor problem has been given by Domb and Potts[15] and to the Ising problem with general spin by Sykes.[14]

The constraints are best exploited by counting only perturbations with $r \geqslant s$, which correspond to configurations most easily counted as relatively few of them are separated. The counting of the more difficult separated configurations is thus avoided. The number of constraints can be increased to $(s + 1)$ by employing the high-temperature specific-heat expansion (Domb[12]) for zero field and to $(s + 2)$ by employing the high-temperature susceptibility expansion (Sykes[14,16]). On a close-packed lattice the method would seem the most effective so far given for deriving the successive $L_s(u)$. We give in Appendix III, the first six $L(u)$ for the face-centered cubic and the first eight $L(u)$ for the triangular lattice which we have derived in this way.

The amount of work involved in deriving the successive $L(u)$ increases rapidly with s. It can be shown by a more detailed analysis of the method of topological breakdown that to calculate $L_s(u)$ it is sufficient to know the number of multiply-connected[17] perturbations with s spins on the lattice considered. This result can be obtained more directly in another way by using the Ursell–Mayer formalism and this approach can be developed as an alternative method for obtaining the $L(u)$. We shall not describe the method since this has been adequately done by Rushbrooke and Scoins[18,19] and Domb and Hiley.[20] Although of great theoretical interest, the Mayer method has not so far led to any easy method of calculating the contributions from the more complex perturbations. A table of the multiply-connected perturbations with up to eight spins (on a loose-packed lattice) is given by Rushbrooke and Scoins[19] and is relatively difficult to provide. We give in Sec. 4, a method which exploits the fact that what is actually required is the numerical value of each $[r; s]$ and that a topological description, complete or partial, is not necessary.

[12] C. Domb, Proc. Roy. Soc. (London) **A199**, 199 (1949).
[13] A. J. Wakefield, Proc. Cambridge Phil. Soc. **47**, 799 (1951).
[14] M. F. Sykes, thesis, Oxford (1956) (unpublished).
[15] C. Domb and R. B. Potts, Proc. Roy. Soc. (London) **A210**, 125 (1951).
[16] M. F. Sykes, J. Math. Phys. **2**, 52 (1961).
[17] A multiply-connected configuration is a connected configuration without articulation points. An articulation point is a point which, if omitted, would cause the configuration to fall into two disconnected parts.
[18] G. S. Rushbrooke and H. I. Scoins, Proc. Roy. Soc. (London) **A230**, 74 (1955).
[19] G. S. Rushbrooke and H. I. Scoins, J. Math. Phys. **3**, 176 (1962).
[20] C. Domb and B. J. Hiley, Proc. Roy. Soc. (London) **A268**, 506 (1962).

3. THE LOW-TEMPERATURE ENUMERATIVE PROBLEM FOR AN ANTIFERROMAGNET

In this section, we consider the antiferromagnetic problem for those lattices which can be decomposed into two equivalent sublattices. We shall denote these two sublattices by A and B and to avoid fractions it is convenient to use N for the number of A or B sites and thus to work with a $2N$ site lattice. (For the antiferromagnet J is negative and we shall write $J' = -J$.) The lowest energy state for small fields is now one of antiparallel ordering in which each A spin is in the opposite state to its nearest neighbors all of which are B spins. If such an ordered state is perturbed by the overturning of s A-spins and t B-spins with r nearest-neighbor links between them the resultant gain in energy is now

$$2[q(s+t) - 2r]J' + 2msH - 2mtH, \qquad (3.1)$$

where we have supposed that the A sublattice is ordered in the direction of the external field.

If there is no applied field (3.1) is identical with (2.1) and we have the well-known result that the configurational problem for a loose-packed Ising antiferromagnet in the absence of an applied field is isomorphic with the ferromagnetic one. It is implicit in (3.1) that $2J'$ now denotes the energy gained if two first-neighbor spins change from *antiparallel* to parallel position. To avoid confusion we shall follow Domb and introduce new variables

$$y = \exp(-2J'/kT), \qquad w = y^2. \qquad (3.2)$$

The energy per spin of the ground state is now simply $-\frac{1}{2}qJ'$ and in place of (2.5) we write

$$F = -\tfrac{1}{2}qJ' - kT \ln \Lambda^a(\mu, w). \qquad (3.3)$$

In the absence of a field the expansion valid near $T = 0$ will be

$$\ln \Lambda^a = \sum_{\text{all } s+t,r} [s+t; r] w^{\frac{1}{2}q(s+t)-r}, \qquad (3.4)$$

and the coefficients will be term by term identical with (2.6) for $\mu = 1$.

In the presence of an applied field this isomorphism is destroyed. We shall find it convenient to modify the ferromagnetic problem to retain a formal isomorphism in the expansions. This isomorphism will not be a physical one since the power series we shall derive will have different regions of validity.

Suppose that for a ferromagnet with two sublattices A and B the spins on the A sublattice have moment m_A and those on the B sublattice m_B and we write

$$\exp(-2m_AH/kT) = \mu, \qquad \exp(-2m_BH/kT) = \nu. \qquad (3.5)$$

The perturbation problem is now more complex since we must include in our description of a disturbed state the distribution of overturned spins between the two sublattices. Denoting the linear part of the total number of ways of choosing s A-sites, t B-sites with r first-neighbor bonds between them by $[s, t; r]$ we require formally

$$\ln \Lambda = \sum_{\text{all } s,t,r} [s, t; r] u^{\frac{1}{2}qs+\frac{1}{2}qt-r} \mu^s \nu^t. \qquad (3.6)$$

For the antiferromagnetic problem we see from (3.1) that the Boltzmann factor is

$$w^{\frac{1}{2}qs+\frac{1}{2}qt-r} \mu^s \mu^{-t}. \qquad (3.7)$$

Thus, for a particular choice of $(s+t)$ and r we obtain as the coefficient of $w^{\frac{1}{2}qs+\frac{1}{2}qt-r}$ a range of powers of μ from μ^{s+t} to μ^{-s-t}. The presence of inverse powers of μ alters the whole character of the expansion since when μ is small $1/\mu$ is large and the converse. The development is therefore best thought of as an expansion in w for fixed μ. A formal isomorphism with (3.6) is obtained by setting $\nu = 1/\mu$, $u = w$. The required expansion is simply

$$\sum_{\text{all } s,t,r} [s, t; r] w^{\frac{1}{2}qs+\frac{1}{2}qt-r} \mu^s \mu^{-t}. \qquad (3.8)$$

Expansions of this type have been given by Brooks and Domb[21] for the simple quadratic lattice and by Wakefield[13] for the simple cubic lattice. Both these authors have used the variable μ only and this is equivalent to writing

$$\mu^s \mu^{-t} = \mu^{s-t}. \qquad (3.9)$$

The treatment in this section, which introduces an isomorphic ferromagnetic problem, retains in the antiferromagnetic expansion information on the distribution of perturbed spins between the two sublattices. This information can be exploited to develop extrapolation techniques. In particular it enables the method of metastable approximations (Domb and Sykes[22]) to be applied to the anti-

[21] J. E. Brooks and C. Domb, Proc. Roy. Soc. (London) **A207**, 343 (1951).

[22] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A235**, 247 (1956).

ferromagnetic problem. Also, so long as the distinction between μ and ν is retained, generalized constraints between the $[s, t; r]$ can be established along the lines used for the simple ferromagnetic problem and these constraints can be used to extend the data. We shall not describe these constraints as we shall propose in the next section an alternative method for deriving the polynomials for the sublattice ferromagnetic problem ($L_{s,t}$) defined by

$$L_{s,t}(u) = \sum_{\text{all } r} [s, t; r] u^{\frac{1}{2}qs + \frac{1}{2}qt - r}. \tag{3.10}$$

The quantities $[s, t; r]$ can be obtained by direct enumeration by an obvious extension of the method of topological breakdown. For example the values, on the body-centered cubic, of [8, 0; 9], [7, 1; 9], [6, 2; 9], [5, 3; 9], [4, 4; 9] can be found by constructing a more detailed description of the perturbations shown in Fig. 1. For connected configurations this presents no special difficulty but the calculation of the distribution of the separated configurations on the two sublattices is often tedious and liable to error.

4. PARTIAL GENERATING FUNCTIONS FOR $[s, t; r]$

In previous sections we have shown that the derivation of low-temperature expansions can be made to depend on the quantities $[s, t; r]$. Defining a generating function F by

$$F(X, Y, b) = \sum_{s,t,r} [s, t; r] X^s Y^t b^r, \tag{4.1}$$

a knowledge of F would be equivalent to a complete solution of the problem. We shall derive in this section partial generating functions which are equivalent to the solution of the problem when the number of overturned spins on one sublattice is held constant. Owing to the symmetric equivalence of the two sublattices a knowledge of the first n partial generating functions enables the values of all $[s, t; r]$ with $s + t \leq 2n + 1$ to be derived. Explicitly we write

$$F(X, Y, b) = \sum_{\lambda} Y^{\lambda} F_{\lambda}(X, b), \tag{4.2}$$

$$F_{\lambda}(X, b) = \sum_{s,r} [s, \lambda; r] X^s b^r. \tag{4.3}$$

We now take as a specific example the body-centered cubic on which as we have seen the configurational problem is relatively complicated. The first partial generating function, F_0, corresponds to configurations for which all the sites are on the A sublattice. Such sites cannot be neighbors of one another and therefore $r = 0$ always. We may choose an A site on an infinite lattice of $2N$ sites in N ways, and then another in $(N - 1)$ ways and so on to obtain each selection of s sites $s!$ times. $[s, 0; 0]$ is, therefore, the coefficient of N in

$$N(N - 1)(N - 2) \cdots (N - s + 1)/s! \quad \text{or} \quad (-1)^{s+1}/s. \tag{4.4}$$

The function F_0 is thus simply

$$F_0(X, b) = \ln (1 + X). \tag{4.5}$$

If all the sites but one are A-sites we first choose the B-site (N ways) and observe that it casts a "shadow" on the eight neighboring A-sites in the sense that if any one of these is now selected a nearest-neighbor bond will be formed. If we choose α A-sites from the eight sites in the "shadow" and β A-sites from the remaining $(N - 8)$ sites we shall obtain α bonds in

$$\binom{8}{\alpha}(N - 8)(N - 9) \cdots (N - 8 - \beta + 1)/\beta! \tag{4.6}$$

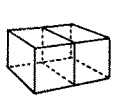
ways. The appropriate term of the expansion of F_1 is, therefore, the term linear in N in this, or

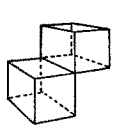
$$(Xb)^{\alpha} X^{\beta} \binom{8}{\alpha}\binom{-8}{\beta} \tag{4.7}$$

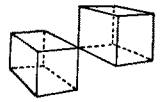
and, therefore,

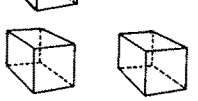
$$F_1(X, b) = (1 + bX)^8 (1 + X)^{-8}. \tag{4.8}$$

To derive the next partial generating function we observe that the two B-sites each cast a "shadow" of eight sites (in the form of a cube) and that these shadows may overlap. The two sublattices on the body-centered cubic form simple cubic lattices and the possible overlappings of the two "shadows" correspond to the various ways in which two cubes may be chosen on a simple cubic lattice. There are four distinct cases:

(a)  Face-to-face $(3N)$

(b)  Edge-to-edge $(6N)$

(c)  Corner-to-corner $(4N)$

(d)  Separated $(\frac{1}{2}N^2 - 13\frac{1}{2}N)$.

(4.9)

In (a) the two cubes have one face in common which means that only 12 A-sites are shaded by the 2 B-sites. Of these 12 sites the 4 on the common face will create two bonds if chosen since they are adjacent to both B-sites. The appropriate generating function is now

$$(1 + bX)^8(1 + b^2X)^4(1 + X)^{-12}. \tag{4.10}$$

Each of the three remaining cases can be treated similarly and on multiplying up by their respective occurrences we obtain

$$\begin{aligned} F_2(X, b) &= 3(1 + bX)^8(1 + b^2X)^4(1 + X)^{-12} \\ &+ 6(1 + bX)^{12}(1 + b^2X)^2(1 + X)^{-14} \\ &+ 4(1 + bX)^{14}(1 + b^2X)(1 + X)^{-15} \\ &- 13\tfrac{1}{2}(1 + bX)^{16}(1 + X)^{-16}. \end{aligned} \tag{4.11}$$

Expressions such as (4.11) are relatively cumbersome and we observe that the general term in $F_n(X, b)$ will be some multiple of

$$\begin{aligned} &(1 + bX)^{\alpha}(1 + b^2X)^{\beta}(1 + b^3X)^{\gamma} \cdots \\ &\qquad /(1 + X)^{\alpha+\beta+\gamma+\cdots} \end{aligned} \tag{4.12}$$

and we shall denote this by

$$(\lambda, \alpha, \beta, \gamma, \cdots), \quad \lambda = \alpha + \beta + \gamma + \cdots, \tag{4.13}$$

which is simpler and forms a convenient "code" for supplying data of this type to an electronic computor. We shall close the bracket when factors to the right terminate but zeros will occur in the code if any factors are missing in the sequence.

On the body-centered cubic the determination of the next two partial generating functions F_3 and F_4 is now reduced to the counting and classifying of all the possible ways of selecting three and four cubes on the simple cubic lattice and determining the respective "codes" of each configuration. This combinatorial problem is closely related to the Ising problem on the simple cubic with first-, second-, and third-neighbor interactions. Referring again to (4.9) the $3N$ arrangements face-to-face correspond to the $3N$ first-neighbor interactions, the $6N$ edge-to-edge correspond to the $6N$ second-neighbor interactions (these form a face-centered cubic lattice), and the $4N$ corner-to-corner correspond to the $4N$ third-neighbor interactions (these form a body-centered cubic lattice). We have exploited this isomorphism to classify and count the 13 combinations of 3 cubes and the 80 combinations of 4 cubes and so derive the next two partial generating functions. This suffices to determine the first nine low-temperature polynomials $L(u)$ of (2.7) for this lattice. The results can be expressed compactly in the form of the codes as:

$$\begin{aligned} F_1 &= 1(8, 8), \\ F_2 &= 3(12, 8, 4) + 6(14, 12, 2) \\ &\quad + 4(15, 14, 1) - 13\tfrac{1}{2}(16, 16), \\ F_3 &= 3(16, 8, 8) + 12(16, 10, 4, 2) + 24(18, 12, 6) \\ &\quad + 24(18, 13, 4, 1) + 24(19, 14, 5) \\ &\quad + 8(19, 15, 3, 1) - 66(20, 16, 4) + 72(21, 18, 3) \\ &\quad - 224(22, 20, 2) - 184(23, 22, 1) + 307\tfrac{1}{3}(24, 24), \\ F_4 &= 3(18, 8, 8, 0, 2) + 3(20, 8, 12) \\ &\quad + 24(20, 10, 8, 2) + 24(20, 12, 4, 4) \\ &\quad + 24(20, 12, 5, 2, 1) + 8(20, 13, 3, 3, 1) \\ &\quad + 6(21, 12, 8, 0, 1) + 24(21, 13, 6, 1, 1) \\ &\quad + 48(22, 12, 10) + 72(22, 13, 8, 1) \\ &\quad + 132(22, 14, 6, 2) + 96(22, 15, 4, 3) \\ &\quad + 60(23, 14, 9) + 24(23, 15, 7, 1) \\ &\quad + 168(23, 16, 5, 2) + 2(23, 16, 6, 0, 1) \\ &\quad - 115\tfrac{1}{2}(24, 16, 8) + 312(24, 17, 6, 1) \\ &\quad - 444(24, 18, 4, 2) + 504(25, 18, 7) \\ &\quad + 432(25, 19, 5, 1) - 1594(26, 20, 6) \\ &\quad - 1104(26, 21, 4, 1) - 1116(27, 22, 5) \\ &\quad - 424(27, 23, 3, 1) + 1479(28, 24, 4) \\ &\quad - 5724(29, 26, 3) + 7962(30, 28, 2) \\ &\quad + 7836(31, 30, 1) - 8721\tfrac{3}{4}(32, 32). \end{aligned} \tag{4.14}$$

From (4.14) we can obtain, by expanding and picking out the terms, complete information on $[s, t; r]$ for all $s + t \leq 9$. For example to derive the antiferromagnetic breakdown of the perturbations in Fig. 1. we require the coefficient of b^9 for all $s + t = 8$ and this is found to be

$$\begin{aligned} &384X^6Y^2 + 17632X^5Y^3 + 46672X^4Y^4 \\ &\quad + 17632X^3Y^5 + 384X^2Y^6. \end{aligned} \tag{4.15}$$

On adding these coefficients together we obtain

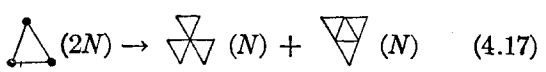
$$\begin{aligned} [8; 9] &= 82704 \quad \text{on} \quad 2N \text{ sites}, \\ &= 41352 \quad \text{on} \quad N \text{ sites}. \end{aligned} \tag{4.16}$$

The method can be applied to any loose-packed lattice and we shall in general find that each A-site or B-site casts a "shadow" conveniently thought of as a solid figure formed by the first-neighbor shell. These shadows must be classified for their possible overlappings and for this purpose it is convenient to study another partially isomorphic Ising problem which may be one involving more than near-neighbor interactions as we have seen in our example. The isomorphism is not complete in the sense that the coding rules are not always simply related to the corresponding Ising configuration. It is, however, possible to code most of the simple lattices with equivalent sites and bonds from information given on the corresponding "shadow lattice." We summarize these in Table I.

TABLE I. Loose-packed lattices and their respective "shadows."

Lattice	Shadow	Shadow lattice
Honeycomb	Triangle	Triangular lattice
Simple quadratic	Square	Simple quadratic lattice with first and second neighbors
Diamond	Tetrahedron	Face-centered cubic lattice
White tin	Tetrahedron	Close-packed hexagonal
Simple cubic	Octahedron	Face-centered cubic lattice with first and second neighbors
Body-centered cubic	Cube	Simple cubic lattice with first, second, and third neighbors

The honeycomb and diamond lattices lead to first-neighbor shadow lattices. On the honeycomb each A-spin casts a triangular shadow of B-spins and any pair of these triangles, if they overlap at all, can only have one point in common. Each triangle is surrounded by six others the over-all topological linkage of possible contacts being a triangular lattice. A choice of say three triangles on the honeycomb lattice corresponds to a choice of three sites on this triangular lattice. Further if any pair of triangles touch, the corresponding configuration on the triangular shadow lattice will contain a first-neighbor bond. To obtain F_3 we need the codes appropriate to all the possible choices of three spins on the triangular lattice. These choices are listed in Appendix I. The codes are not difficult to provide and we observe that a triangle of spins can correspond to two possible overlappings of three triangles in accordance with the scheme



(4.17)

by symmetry and the appropriate coding will therefore be

$$1(7, 6, 0, 1) + 1(6, 3, 3). \tag{4.18}$$

We give in the last two columns of Appendix I the codes for the honeycomb and diamond lattices. To obtain the contribution to F each entry should be multiplied by the corresponding occurrence factor. In a similar way the codes for the white tin lattice can be derived from data on the close-packed hexagonal lattice but as this latter is not a bravais lattice, the corresponding "white tin code" is relatively complicated.

The simple cubic lattice leads to the problem of choosing octahedra and the shadow lattice is the face-centered cubic with second-neighbor bonds. A first-neighbor bond corresponds to two octahedra edge-to-edge and a second-neighbor bond to two octahedra corner-to-corner. To obtain F_5 every arrangement of five octahedra must be classified. Among the most difficult are the separated arrangements such as, for instance, the contribution from five octahedra, no one touching any other. This is just the number of completely separated five spins for the Ising problem (face-centered cubic with second neighbors) on the shadow lattice and may be deduced by using the constraints already referred to in Sec. 2. In this we have been assisted by N. Dalton who has derived the first five low-temperature polynomials for this second-neighbor problem.

In Appendix II, we give the partial generating functions we have derived.

5. APPLICATIONS

From the partial generating functions in Appendix II the complete free-energy expansion for the two sublattice ferromagnet can be derived for all $s + t \leq 2n + 1$ where F_n is the last partial generating function available. We shall not quote these expansions explicitly because of the extent of the data. The manipulation of such expansions is only conveniently done on a computer and for this purpose the coded partial generating functions would seem to provide a convenient form of the data. Each new partial generating function when expanded must reproduce the earlier terms correctly and this fact provides a most useful test of the correctness of the underlying enumeration.

The partial generating functions up to F_n determine the ferromagnetic polynomials up to $L_{2n+1}(u)$ and we quote these in Appendix III. For

the simple quadratic lattice we have obtained 13 polynomials and the first 10 are in agreement with those given by Sykes.[16] For the triangular lattice we give 8 and the first 6 are in agreement with Domb and Sykes.[22] For the face-centered cubic we have done no more than verify the results of Domb and Hiley.[20] We give 13 polynomials for the honeycomb and diamond lattices and these are new. For the simple cubic we give 11 the first 8 being in agreement with Domb and Sykes.[22] For the body-centered cubic we give 9 the first 8 being in agreement with Rushbrooke and Scoins[19] apart from an obvious misprint. It is still feasible in most cases to obtain further generating functions without undue labor and we are continuing with this work. These polynomials $L(u)$ provide an expansion of the free energy grouped in powers of μ (μ grouping).

For some studies, in particular those of the spontaneous magnetization and the specific heat in zero field, it is convenient to group in powers of u (u grouping). To extend the u grouping it is an advantage to know the leading terms in higher $L(u)$. These extra coefficients can be obtained by the method of topological breakdown or alternatively by enumerating only those 'codes' whose expansion will make a contribution to the required coefficient. We have extended the u grouping by these methods and derived expansions for the configurational free energy in the absence of a field and we give these in Appendix IV. The corresponding expansions for the reduced configurational energy $U(u)$ and the specific heat at constant field C_H can be derived through the defining relations

$$U(u) = 4u\,\partial L/\partial u, \qquad L = \ln \Lambda \tag{5.1}$$

$$C_H/R(\ln u)^2 = \tfrac{1}{4}u\,\partial U/\partial u \tag{5.2}$$

From the same data the reduced spontaneous magnetization $I(u)$ and the low-temperature zero-field ferromagnetic reduced susceptibility $\chi(u)$ can be obtained through the defining relations

$$I(u) = 1 - 2\mu\,\partial L/\partial \mu\,|_{\mu=1}, \tag{5.3}$$

$$\chi(u) = (2\mu\,\partial/\partial\mu)^2 L\,|_{\mu=1}. \tag{5.4}$$

We give the magnetization expansions and the expansions for ln Λ in the absence of a field in Appendix IV.

For the antiferromagnetic problem we have derived the free energy expansion in the form adopted by Brooks and Domb[21] for the simple quadratic lattice and by Wakefield[13] for the simple cubic lattice as

$$\ln \Lambda^a = \sum a_k y^k, \tag{5.5}$$

where each coefficient a_k is a polynomial in powers of μ and $1/\mu$. These must occur symmetrically and it is convenient to write

$$\theta_n = \mu^n + \mu^{-n}. \tag{5.6}$$

We give these antiferromagnetic expansions in Appendix V together with the derived expansions for the corresponding reduced antiferromagnetic zero-field susceptibility $\chi^a(y)$

$$\dot{\chi}^a(y) = (2\mu\,\partial/\partial\mu)^2 L^a\,|_{\mu=1}. \tag{5.7}$$

For the simple quadratic we have added two, and for the simple cubic four, more terms to those available previously. The data for the honeycomb, diamond, and body-centered cubic lattices are new.

As stated in the introduction we shall not make any analysis here of the data we have derived. The data for the two sublattice model is being analyzed in collaboration with Bienenstock[11] with a view to its application to the nonstoichiometric alloy problem. The data for the simple Ising model is being studied in collaboration with Fisher[7] to elucidate the behavior of the magnetization in the presence of a field. We are also extending the calculations outlined in this paper to provide further data. With the recent improvements in extrapolation methods it should be possible eventually to resolve most of the obscurities still extant in our understanding of the physical properties of the three-dimensional Ising model; such as for example the critical behavior of the ferromagnetic susceptibility just below the Curie point and the relationship of this to the specific heat singularity.[23]

ACKNOWLEDGMENTS

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[23] G. S. Rushbrooke, J. Chem. Phys. **39**, 842 (1963).

APPENDIX I. TABLE OF THE PERTURBATIONS OF UP TO FIVE SPINS ON THE TRIANGULAR AND FACE-CENTERED CUBIC LATTICES

Configuration	Coeff. N. Δ lar	Coeff. N. fcc	H.–C. Code	Diamond Code
	+1	+1	(3, 3)	(4, 4)
	+3	+6	(5, 4, 1)	(7, 6, 1)
	$-3\frac{1}{2}$	$-6\frac{1}{2}$	(6, 6)	(8, 8)
	+2	+8	$\frac{1}{2}$(7, 6, 0, 1) $\frac{1}{2}$(6, 3, 3)	$\frac{1}{2}$(9, 6, 3) $\frac{1}{2}$(10, 9, 0, 1)
	+9	+42	(7, 5, 2)	(10, 8, 2)
	−30	−120	(8, 7, 1)	(11, 10, 1)
	$+19\frac{1}{3}$	$+70\frac{1}{3}$	(9, 9)	(12, 12)
	0	+2		$\frac{1}{2}$(10, 4, 6) $\frac{1}{2}$(13, 12, 0, 0, 1)
	+3	+24	(8, 5, 2, 1)	(12, 9, 2, 1)
	0	+3		(12, 8, 4)
	+12	+120	$\frac{1}{2}$(8, 4, 4) $\frac{1}{2}$(9, 7, 1, 1)	$\frac{1}{2}$(12, 8, 4) $\frac{1}{2}$(13, 11, 1, 1)
	+27	+282	(9, 6, 3)	(13, 10, 3)
	+2	+44	(9, 6, 3)	(13, 10, 3)
	−24	−200	$\frac{1}{2}$(10, 9, 0, 1) $\frac{1}{2}$(9, 6, 3)	$\frac{1}{2}$(13, 10, 3) $\frac{1}{2}$(14, 13, 0, 1)
	$-61\frac{1}{2}$	−531	(10, 8, 2)	(14, 12, 2)
	−117	−1122	(10, 8, 2)	(14, 12, 2)
	+288	+2322	(11, 10, 1)	(15, 14, 1)
	$-129\frac{3}{4}$	$-944\frac{1}{4}$	(12, 12)	(16, 16)
	0	+6		(14, 10, 2, 2)
	0	+24		$\frac{1}{2}$(13, 7, 5, 1) $\frac{1}{2}$(15, 12, 2, 0, 1)

Configuration	Coeff. N. Δ lar	Coeff. N. fcc	H.-C. Code	Diamond Code
	+6	+72	$\frac{1}{2}(9, 4, 4, 1)$ $\frac{1}{2}(10, 7, 1, 2)$	$\frac{1}{2}(14, 9, 4, 1)$ $\frac{1}{2}(15, 12, 1, 2)$
	0	+24		$\frac{1}{2}(13, 6, 7)$ $\frac{1}{2}(16, 14, 1, 0, 1)$
	0	−56		$\frac{1}{2}(14, 8, 6)$ $\frac{1}{2}(17, 16, 0, 0, 1)$
	0	+24		$\frac{1}{2}(14, 8, 6)$ $\frac{1}{2}(15, 11, 3, 1)$
	+6	+168	(10, 6, 3, 1)	(15, 11, 3, 1)
	+12	+240		
	+3	+72	(10, 6, 3, 1)	$\frac{1}{6}(14, 8, 6)$ $\frac{2}{3}(15, 11, 3, 1)$ $\frac{1}{6}(16, 14, 0, 2)$
	0	+48		(15, 10, 5)
	+36	+792		
	+24	+576	$\frac{1}{2}(10, 5, 5)$ $\frac{1}{2}(11, 8, 2, 1)$	$\frac{1}{2}(15, 10, 5)$ $\frac{1}{2}(16, 13, 2, 1)$
	0	+96		
	−42	−720	(11, 8, 2, 1)	(16, 13, 2, 1)
	0	−90		(16, 12, 4)
	−96	−1728	$\frac{1}{2}(12, 10, 1, 1)$ $\frac{1}{2}(11, 7, 4)$	$\frac{1}{2}(16, 12, 4)$ $\frac{1}{2}(17, 15, 1, 1)$
	−180	−3792		
	+81	+1902		
	+18	+828	(11, 7, 4)	(16, 12, 4)
	0	+9		
	+252	+4328	$\frac{1}{2}(13, 12, 0, 1)$ $\frac{1}{2}(12, 9, 3)$	$\frac{1}{2}(17, 14, 3)$ $\frac{1}{2}(18, 17, 0, 1)$

Configuration	Coeff. N. Δ lar	Coeff. N. fcc	H.–C. Code	Diamond Code
	−32	−1448		
	−432	−9444	(12, 9, 3)	(17, 14, 3)
	−468	−9732		
	+1350	+24006	(13, 11, 2)	(18, 16, 2)
	+1287	+25284	(13, 11, 2)	(18, 16, 2)
	−2796	−45792	(14, 13, 1)	(19, 18, 1)
	$+971\frac{1}{5}$	$+14303\frac{1}{5}$	(15, 15)	(20, 20)

APPENDIX II. PARTIAL GENERATING FUNCTIONS

Honeycomb Lattice

$$F_1 = 1(3, 3),$$

$$F_2 = 3(5, 4, 1) - 3\tfrac{1}{2}(6, 6),$$

$$F_3 = 1(6, 3, 3) + 9(7, 5, 2) + 1(7, 6, 0, 1) - 30(8, 7, 1) + 19\tfrac{1}{3}(9, 9),$$

$$F_4 = 6(8, 4, 4) + 3(8, 5, 2, 1) + 17(9, 6, 3) + 6(9, 7, 1, 1) - 178\tfrac{1}{2}(10, 8, 2) - 12(10, 9, 0, 1) + 288(11, 10, 1) - 129\tfrac{3}{4}(12, 12),$$

$$F_5 = 3(9, 4, 4, 1) + 30(10, 5, 5) + 21(10, 6, 3, 1) + 3(10, 7, 1, 2) - 39(11, 7, 4) - 12(11, 8, 2, 1) - 806(12, 9, 3) - 138(12, 10, 1, 1) + 2637(13, 11, 2) + 126(13, 12, 0, 1) - 2796(14, 13, 1) + 971\tfrac{1}{5}(15, 15),$$

$$F_6 = 1(10, 3, 6, 1) + 3(11, 4, 7) + 21(11, 5, 5, 1) + 12(11, 6, 3, 2) + 131\tfrac{1}{2}(12, 6, 6) + 75(12, 7, 4, 1) + 21(12, 8, 2, 2) + 1(12, 9, 0, 3) - 726(13, 8, 5) - 400(13, 9, 3, 1) - 45(13, 10, 1, 2) - 2353\tfrac{1}{2}(14, 10, 4) - 594(14, 11, 2, 1) - 9\tfrac{1}{2}(14, 12, 0, 2) + 18097(15, 12, 3) + 2217(15, 13, 1, 1) - 34920(16, 14, 2) - 1290(16, 15, 0, 1) + 27555(17, 16, 1) - 7796\tfrac{2}{3}(18, 18).$$

Simple Quadratic Lattice

$$F_1 = 1(4, 4),$$

$$F_2 = 2(6, 4, 2) + 2(7, 6, 1) - 4\tfrac{1}{2}(8, 8),$$

$$F_3 = 2(8, 4, 4) + 4(8, 5, 2, 1) + 8(9, 6, 3) - 18(10, 8, 2) - 28(11, 10, 1) + 32\tfrac{1}{3}(12, 12),$$

$$F_4 = 1(9, 4, 4, 0, 1) + 2(10, 4, 6) + 8(10, 5, 4, 1) + 8(10, 6, 2, 2) + 16(11, 6, 5) + 20(11, 7, 3, 1) - 24(12, 8, 4) - 60(12, 9, 2, 1) - 190(13, 10, 3) + 140(14, 12, 2) + 362(15, 14, 1) - 283\tfrac{1}{4}(16, 16),$$

$$F_5 = 8(11, 5, 4, 1, 1) + 2(12, 4, 8) + 12(12, 5, 6, 1) + 28(12, 6, 4, 2) + 4(12, 6, 5, 0, 1) + 12(12, 7, 2, 3) + 1(12, 8, 0, 4) + 24(13, 6, 7) + 84(13, 7, 5, 1) + 48(13, 8, 3, 2) - 16(13, 8, 4, 0, 1) - 208(14, 9, 4, 1) - 144(14, 10, 2, 2) - 592(15, 10, 5) - 564(15, 11, 3, 1) - 160(16, 12, 4) + 804(16, 13, 2, 1) + 3296(17, 14, 3) - 738(18, 16, 2) - 4672(19, 18, 1) + 2771\tfrac{1}{5}(20, 20),$$

$$F_6 = 2(12, 4, 6, 0, 2) + 8(13, 5, 6, 1, 1) + 28(13, 6, 4, 2, 1) + 4(13, 7, 2, 3, 1) + 2(14, 4, 10) + 16(14, 5, 8, 1) + 66(14, 6, 6, 2) + 8(14, 6, 7, 0, 1) + 72(14, 7, 4, 3) + 40(14, 7, 5, 1, 1) + 24(14, 8, 2, 4) + 32(15, 6, 9) + 188(15, 7, 7, 1) + 318(15, 8, 5, 2) - 22(15, 8, 6, 0, 1) + 84(15, 9, 3, 3) - 152(15, 9, 4, 1, 1) + 8(15, 10, 1, 4) + 62(16, 8, 8) - 208(16, 9, 6, 1) - 910(16, 10, 4, 2) - 130(16, 10, 5, 0, 1) - 252(16, 11, 2, 3) - 21(16, 12, 0, 4) - 1202(17, 10, 7)$$

$$- 3732(17, 11, 5, 1) - 1472(17, 12, 3, 2) + 222(17, 12, 4, 0, 1) - 2617\tfrac{1}{3}(18, 12, 6)$$
$$+ 2780(18, 13, 4, 1) + 2128(18, 14, 2, 2) + 12914(19, 14, 5) + 11500(19, 15, 3, 1) + 13142(20, 16, 4)$$
$$- 10604(20, 17, 2, 1) - 50455\tfrac{1}{3}(21, 18, 3) - 3634(22, 20, 2) + 60860(23, 22, 1) - 29096\tfrac{1}{2}(24, 24).$$

Diamond Lattice

$$F_1 = 1(4, 4),$$
$$F_2 = 6(7, 6, 1) - 6\tfrac{1}{2}(8, 8),$$
$$F_3 = 4(9, 6, 3) + 42(10, 8, 2) + 4(10, 9, 0, 1) - 120(11, 10, 1) + 70\tfrac{1}{3}(12, 12),$$
$$F_4 = 1(10, 4, 6) + 63(12, 8, 4) + 24(12, 9, 2, 1) + 226(13, 10, 3) + 60(13, 11, 1, 1)$$
$$+ 1(13, 12, 0, 0, 1) - 1653(14, 12, 2) - 100(14, 13, 0, 1) + 2322(15, 14, 1) - 944\tfrac{1}{4}(16, 16),$$
$$F_5 = 12(13, 6, 7) + 12(13, 7, 5, 1) - 4(14, 8, 6) + 36(14, 9, 4, 1) + 6(14, 10, 2, 2)$$
$$+ 780(15, 10, 5) + 468(15, 11, 3, 1) + 36(15, 12, 1, 2) + 12(15, 12, 2, 0, 1) - 111(16, 12, 4)$$
$$+ 12(16, 13, 2, 1) + 12(16, 14, 0, 2) + 12(16, 14, 1, 0, 1) - 18460(17, 14, 3) - 2760(17, 15, 1, 1)$$
$$- 28(17, 16, 0, 0, 1) + 49290(18, 16, 2) + 2164(18, 17, 0, 1) - 45792(19, 18, 1) + 14303\tfrac{1}{3}(20, 20),$$
$$F_6 = 24(15, 7, 7, 1) + 12(15, 8, 5, 2) + 156(16, 8, 8) + 208(16, 9, 6, 1) + 60(16, 10, 4, 2)$$
$$+ 6(16, 10, 5, 0, 1) + 1(16, 12, 0, 4) - 72(17, 10, 7) + 624(17, 11, 5, 1) + 360(17, 12, 3, 2)$$
$$+ 48(17, 12, 4, 0, 1) + 12(17, 13, 1, 3) + 12(17, 13, 2, 1, 1) + 8588(18, 12, 6) + 5568(18, 13, 4, 1)$$
$$+ 690(18, 14, 2, 2) + 192(18, 14, 3, 0, 1) + 16(18, 15, 0, 3) + 24(18, 15, 1, 1, 1) - 30318(19, 14, 5)$$
$$- 15356(19, 15, 3, 1) - 906(19, 16, 1, 2) - 258(19, 16, 2, 0, 1) - 154464(20, 16, 4) - 34752(20, 17, 2, 1)$$
$$- 782(20, 18, 0, 2) - 660(20, 18, 1, 0, 1) + 816900(21, 18, 3) + 90240(21, 19, 1, 1) + 646(21, 20, 0, 0, 1)$$
$$- 1329240(22, 20, 2) - 45628(22, 21, 0, 1) + 922152(23, 22, 1) - 234103\tfrac{1}{6}(24, 24).$$

Simple Cubic Lattice

$$F_1 = 1(6, 6),$$
$$F_2 = 6(10, 8, 2) + 3(11, 10, 1) - 9\tfrac{1}{2}(12, 12),$$
$$F_3 = 8(13, 9, 3, 1) + 30(14, 10, 4) + 12(14, 11, 2, 1) + 48(15, 12, 3)$$
$$- 153(16, 14, 2) - 96(17, 16, 1) + 151\tfrac{1}{3}(18, 18),$$
$$F_4 = 12(16, 10, 4, 2) + 12(16, 10, 5, 0, 1) + 2(16, 12, 0, 4) + 72(17, 11, 5, 1)$$
$$+ 48(17, 12, 3, 2) + 3(17, 12, 4, 0, 1) + 164(18, 12, 6) + 216(18, 13, 4, 1)$$
$$+ 24(18, 14, 2, 2) + 480(19, 14, 5) - 140(19, 15, 3, 1) - 1428(20, 16, 4)$$
$$- 444(20, 17, 2, 1) - 2689(21, 18, 3) + 3808\tfrac{1}{2}(22, 20, 2) + 2865(23, 22, 1) - 3005\tfrac{3}{4}(24, 24),$$
$$F_5 = 6(18, 9, 8, 0, 0, 1) + 24(19, 11, 5, 3) + 48(19, 11, 6, 1, 1) + 24(19, 13, 2, 3, 1) + 132(20, 12, 6, 2)$$
$$+ 96(20, 12, 7, 0, 1) + 120(20, 13, 4, 3) + 144(20, 13, 5, 1, 1) + 36(20, 14, 2, 4) + 624(21, 13, 7, 1)$$
$$+ 840(21, 14, 5, 2) + 144(21, 14, 6, 0, 1) + 168(21, 15, 3, 3) + 24(21, 15, 4, 1, 1) + 24(21, 16, 1, 4)$$
$$+ 966(22, 14, 8) + 2652(22, 15, 6, 1) + 618(22, 16, 4, 2) - 444(22, 16, 5, 0, 1) + 36(22, 17, 2, 3)$$
$$- 77(22, 18, 0, 4) + 4128(23, 16, 7) - 1932(23, 17, 5, 1) - 1728(23, 18, 3, 2) - 126(23, 18, 4, 0, 1)$$
$$- 10742(24, 18, 6) - 13788(24, 19, 4, 1) - 1104(24, 20, 2, 2) - 42096(25, 20, 5) - 172(25, 21, 3, 1)$$
$$+ 46647(26, 22, 4) + 14256(26, 23, 2, 1) + 114328(27, 24, 3)$$
$$- 95520(28, 26, 2) - 85884(29, 28, 1) + 67528\tfrac{1}{5}(30, 30).$$

APPENDIX III. FERROMAGNETIC POLYNOMIALS $L(u)$

Triangular

$$L_1 = u^3,$$
$$L_2 = 3u^5 - 3\tfrac{1}{2}u^6,$$
$$L_3 = 2u^6 + 9u^7 - 30u^8 + 19\tfrac{1}{3}u^9,$$
$$L_4 = 3u^7 + 12u^8 + 5u^9 - 178\tfrac{1}{2}u^{10} + 288u^{11} - 129\tfrac{3}{4}u^{12},$$
$$L_5 = 6u^8 + 21u^9 + 18u^{10} - 177u^{11} - 680u^{12} + 2637u^{13} - 2796u^{14} + 971\tfrac{1}{5}u^{15},$$
$$L_6 = 14u^9 + 42u^{10} + 33u^{11} - 278u^{12} - 1320u^{13} - 136\tfrac{1}{2}u^{14} + 16807u^{15} - 34920u^{16} + 27555u^{17} - 7796\tfrac{2}{3}u^{18},$$

$$L_7 = u^9 + 30u^{10} + 105u^{11} + 24u^{12} - 564u^{13} - 2682u^{14} - 3007u^{15} + 21168u^{16} + 63870u^{17} - 307476u^{18} + 437997u^{19} - 275184u^{20} + 65718\tfrac{1}{7}u^{21},$$

$$L_8 = 6u^{10} + 69u^{11} + 227u^{12} + 120u^{13} - 1822\tfrac{1}{2}u^{14} - 5313u^{15} - 8859u^{16} + 30825u^{17} + 165894\tfrac{1}{2}u^{18} - 58668u^{19} - 1907846\tfrac{1}{4}u^{20} + 4905025u^{21} - 5324130u^{22} + 2778678u^{23} - 574205\tfrac{7}{8}u^{24}.$$

Face-Centered Cubic

$$L_1 = u^6,$$

$$L_2 = 6u^{11} - 6\tfrac{1}{2}u^{12},$$

$$L_3 = 8u^{15} + 42u^{16} - 120u^{17} + 70\tfrac{1}{3}u^{18},$$

$$L_4 = 2u^{18} + 24u^{19} + 123u^{20} + 126u^{21} - 1653u^{22} + 2322u^{23} - 944\tfrac{1}{4}u^{24},$$

$$L_5 = 30u^{22} + 96u^{23} + 448u^{24} + 792u^{25} - 2871u^{26} - 16296u^{27} + 49290u^{28} - 45792u^{29} + 14303\tfrac{1}{3}u^{30},$$

$$L_6 = u^{24} + 30u^{25} + 168u^{26} + 776u^{27} + 1212u^{28} + 3930u^{29} - 6904u^{30} - 65070u^{31} - 64224u^{32} + 771272u^{33} - 1329240u^{34} + 922152u^{35} - 234103\tfrac{1}{6}u^{36}.$$

Honeycomb

$$L_1 = z^3,$$

$$L_2 = 1\tfrac{1}{2}z^4 - 2z^6,$$

$$L_3 = 3z^5 - 9z^7 + 6\tfrac{1}{2}z^9,$$

$$L_4 = 7z^6 - 33\tfrac{3}{4}z^8 + 51z^{10} - 24\tfrac{1}{2}z^{12},$$

$$L_5 = 18z^7 - 121z^9 + 288z^{11} - 291z^{13} + 106\tfrac{1}{5}z^{15},$$

$$L_6 = \tfrac{1}{2}z^6 + 46\tfrac{1}{2}z^8 - 421\tfrac{1}{2}z^{10} + 1400\tfrac{1}{2}z^{12} - 2212\tfrac{1}{2}z^{14} + 1681\tfrac{1}{2}z^{16} - 495\tfrac{1}{6}z^{18},$$

$$L_7 = 3z^7 + 116z^9 - 1422z^{11} + 6225z^{13} - 13647z^{15} + 16128z^{17} - 9831z^{19} + 2428\tfrac{1}{7}z^{21},$$

$$L_8 = 13\tfrac{1}{2}z^8 + 270z^{10} - 4640\tfrac{1}{2}z^{12} + 25938z^{14} - 74083\tfrac{7}{8}z^{16} + 120844z^{18} - 114043\tfrac{1}{4}z^{20} + 58056z^{22} - 12353\tfrac{3}{4}z^{24},$$

$$L_9 = 55z^9 + 534z^{11} - 14583z^{13} + 102659z^{15} - 367878z^{17} + 776475z^{19} - 1007093z^{21} + 790929z^{23} - 345741z^{25} + 64643\tfrac{1}{6}z^{27},$$

$$L_{10} = 1\tfrac{1}{2}z^8 + 199\tfrac{1}{2}z^{10} + 639\tfrac{1}{2}z^{12} - 43740z^{14} + 388501\tfrac{1}{2}z^{16} - 1706988\tfrac{1}{2}z^{18} + 4480345\tfrac{4}{5}z^{20} - 7483705\tfrac{1}{2}z^{22} + 8050177z^{24} - 5413245z^{26} + 2073639z^{28} - 345824\tfrac{9}{10}z^{30},$$

$$L_{11} = 12z^9 + 654z^{11} - 1275z^{13} - 123466z^{15} + 1409742z^{17} - 7495464z^{19} + 23835698z^{21} - 49234914z^{23} + 67965699z^{25} - 62427238z^{27} + 36699132z^{29} - 12512061z^{31} + 1883481\tfrac{1}{11}z^{33},$$

$$L_{12} = 67\tfrac{1}{2}z^{10} + 1938\tfrac{1}{4}z^{12} - 13866z^{14} - 319373\tfrac{1}{4}z^{16} + 4905536\tfrac{5}{6}z^{18} - 31390220\tfrac{1}{4}z^{20} + 118851003z^{22} - 295421769\tfrac{1}{4}z^{24} + 502353217\tfrac{1}{2}z^{26} - 590506164\tfrac{3}{4}z^{28} + 473111748z^{30} - 247047660\tfrac{3}{4}z^{32} + 75886312\tfrac{1}{2}z^{34} - 10410769\tfrac{5}{12}z^{36},$$

$$L_{13} = z^9 + 318z^{11} + 5013z^{13} - 70989z^{15} - 711801z^{17} + 16327032z^{19} - 125973077z^{21} + 561454560z^{23} - 1647593244z^{25} + 3356405218z^{27} - 4845906219z^{29} + 4957723473z^{31} - 3521641853z^{33} + 1654028712z^{35} - 462310344z^{37} + 58263200\tfrac{1}{13}z^{39}.$$

Simple Quadratic

$$L_1 = u^2,$$

$$L_2 = 2u^3 - 2\tfrac{1}{2}u^4,$$

$$L_3 = 6u^4 - 16u^5 + 10\tfrac{1}{3}u^6,$$

$$L_4 = u^4 + 18u^5 - 85u^6 + 118u^7 - 52\tfrac{1}{4}u^8,$$

$$L_5 = 8u^5 + 43u^6 - 400u^7 + 926u^8 - 872u^9 + 295\tfrac{1}{5}u^{10},$$

$$L_6 = 2u^5 + 40u^6 + 30u^7 - 1651u^8 + 5992\tfrac{2}{3}u^9 - 9144u^{10} + 6520u^{11} - 1789\tfrac{5}{6}u^{12},$$

$$L_7 = 22u^6 + 136u^7 - 486u^8 - 5664u^9 + 33609u^{10} - 75640u^{11} + 85954u^{12} - 49328u^{13} + 11397\tfrac{1}{7}u^{14},$$

$$L_8 = 6u^6 + 134u^7 + 194\tfrac{1}{2}u^8 - 3986u^9 - 13323u^{10} + 164790u^{11} - 532196\tfrac{1}{2}u^{12} + 867670u^{13} - 785091u^{14} + 377040u^{15} - 75238\tfrac{1}{8}u^{16},$$

$$L_9 = u^6 + 72u^7 + 540u^8 - 1420u^9 - 19786u^{10} + 5112u^{11} + 691734u^{12} - 3282328u^{13} + 7330033u^{14} - 9367653\tfrac{1}{3}u^{15} + 7040042u^{16} - 2906956u^{17} + 510609\tfrac{4}{9}u^{18},$$

$$L_{10} = 30u^7 + 461u^8 + 1144u^9 - 15480u^{10} - 66020u^{11} + 300885\tfrac{1}{2}u^{12} + 2300266u^{13} - 17888832u^{14} + 53980742\tfrac{2}{5}u^{15} - 92320336u^{16} + 97010462u^{17} - 62337864u^{18} + 22576512u^{19} - 3541971u^{20},$$

$$L_{11} = 8u^7 + 310u^8 + 1864u^9 - 3373u^{10} - 91688u^{11} - 69358u^{12} + 2204652u^{13} + 4259359u^{14} - 85259912u^{15} + 353290460u^{16} - 787713256u^{17} + 1092475985u^{18} - 974679560u^{19} + 547000294u^{20} - 176425772u^{21} + 25009987\tfrac{1}{11}u^{22},$$

$$L_{12} = 2u^7 + 151u^8 + 1894u^9 + 3315u^{10} - 53428u^{11} - 383706\tfrac{2}{3}u^{12} + 1032758u^{13} + 10552273u^{14} - 14665400u^{15} - 341367843\tfrac{1}{2}u^{16} + 2067415954u^{17} - 5967607048\tfrac{1}{3}u^{18} + 10581976596u^{19} - 12347150173u^{20} + 9570815133\tfrac{1}{3}u^{21} - 4767367976u^{22} + 1386008952u^{23} - 179211452\tfrac{11}{12}u^{24},$$

$$L_{13} = 68u^8 + 1340u^9 + 7389u^{10} - 20332u^{11} - 350828u^{12} - 965172u^{13} + 10420351u^{14} + 32176924u^{15} - 210691538u^{16} - 1007111904u^{17} + 10753093949u^{18} - 40670308548u^{19} + 90746211502u^{20} - 133748320084u^{21} + 134710804372u^{22} - 92310171884u^{23} + 41333506670u^{24} - 10938421828u^{25} + 1300139553\tfrac{1}{18}u^{26}.$$

Diamond

$$L_1 = u^2,$$

$$L_2 = 2u^3 - 2\tfrac{1}{2}u^4,$$

$$L_3 = 6u^4 - 16u^5 + 10\tfrac{1}{3}u^6,$$

$$L_4 = 22u^5 - 91u^6 + 122u^7 - 53\tfrac{1}{4}u^8,$$

$$L_5 = 91u^6 - 512u^7 + 1054u^8 - 944u^9 + 311\tfrac{1}{5}u^{10},$$

$$L_6 = 2u^6 + 396u^7 - 2877u^8 + 8066\tfrac{2}{3}u^9 - 11058u^{10} + 7442u^{11} - 1971\tfrac{5}{6}u^{12},$$

$$L_7 = 24u^7 + 1746u^8 - 16072u^9 + 57749u^{10} - 107608u^{11} + 110586u^{12} - 59640u^{13} + 13215\tfrac{1}{7}u^{14},$$

$$L_8 = 207u^8 + 7574u^9 - 88765u^{10} + 395018u^{11} - 939367\tfrac{1}{2}u^{12} + 1309590u^{13} - 1076491u^{14} + 484522u^{15} - 92287\tfrac{5}{8}u^{16},$$

$$L_9 = 6u^8 + 1508u^9 + 31365u^{10} - 482136u^{11} + 2607402u^{12} - 7618128u^{13} + 13515382u^{14} - 15044957\tfrac{1}{3}u^{15} + 10305468u^{16} - 3980980u^{17} + 665070\tfrac{4}{9}u^{18},$$

$$L_{10} = u^8 + 102u^9 + 9834u^{10} + 118568u^{11} - 2562436\tfrac{1}{2}u^{12} + 16692444u^{13} - 58481770u^{14} + 126923238\tfrac{2}{5}u^{15} - 179415170u^{16} + 166182038u^{17} - 97571488u^{18} + 33017786u^{19} - 4913147u^{20},$$

$$L_{11} = 16u^9 + 1120u^{10} + 58920u^{11} + 368354u^{12} - 13251196u^{13} + 103918606u^{14} - 429703296u^{15} + 1111277214u^{16} - 1916295528u^{17} + 2250195820u^{18} - 1784298632u^{19} + 916718762u^{20} - 276020892u^{21} + 37030732\tfrac{1}{11}u^{22},$$

$$L_{12} = 198u^{10} + 9894u^{11} + 327231u^{12} + 558252u^{13} - 66199876u^{14} + 629834815\tfrac{1}{3}u^{15} - 3043196788\tfrac{1}{2}u^{16} + 9208521432u^{17} - 18852210871\tfrac{1}{3}u^{18} + 26950755018u^{19} - 27056350183u^{20} + 18753735784\tfrac{2}{3}u^{21} - 8565084633u^{22} + 2323063572u^{23} - 283763845\tfrac{1}{4}u^{24},$$

$$L_{13} = 12u^{10} + 2064u^{11} + 75536u^{12} + 1682888u^{13} - 4273104u^{14} - 316157712u^{15} + 3716643708u^{16} - 20868409268u^{17} + 72935017570u^{18} - 173881731776u^{19} + 294393454158u^{20} - 359264976320u^{21} + 314923472587u^{22} - 193868155232u^{23} + 79693566888u^{24} - 19665127716u^{25} + 2204915717\tfrac{1}{18}u^{26}.$$

Simple Cubic

$$L_1 = u^3,$$

$$L_2 = 3u^5 - 3\tfrac{1}{2}u^6,$$

$$L_3 = 15u^7 - 36u^8 + 21\tfrac{1}{3}u^9,$$

$$L_4 = 3u^8 + 83u^9 - 328\tfrac{1}{2}u^{10} + 405u^{11} - 162\tfrac{3}{4}u^{12},$$

$$L_5 = 48u^{10} + 426u^{11} - 2804u^{12} + 5532u^{13} - 4608u^{14} + 1406\tfrac{1}{5}u^{15},$$

$$L_6 = 18u^{11} + 496u^{12} + 1575u^{13} - 22144\tfrac{1}{2}u^{14} + 64574u^{15} - 84738u^{16} + 53370u^{17} - 13150\tfrac{2}{3}u^{18},$$

$$L_7 = 8u^{12} + 378u^{13} + 3888u^{14} - 1360u^{15} - 157380u^{16} + 674652u^{17} - 1261904u^{18} + 1240035u^{19} - 628236u^{20} + 129919\tfrac{1}{7}u^{21},$$

$$L_8 = u^{12} + 306u^{14} + 4622u^{15} + 22396\tfrac{1}{2}u^{16} - 106113u^{17} - 947582\tfrac{1}{2}u^{18} + 6392769u^{19} - 16362155\tfrac{1}{4}u^{20} + 22521935u^{21} - 17686675\tfrac{1}{2}u^{22} + 7496787u^{23} - 1336290\tfrac{3}{8}u^{24},$$

$$L_9 = 24u^{14} + 127u^{15} + 5544u^{16} + 40050u^{17} + 60804u^{18} - 1368954u^{19} - 3978300u^{20} + 54753064u^{21} - 190517760u^{22} + 348702921u^{23} - 379686836u^{24} + 248294610u^{25} - 90480828u^{26} + 14175534\tfrac{1}{9}u^{27},$$

$$L_{10} = 24u^{15} + 396u^{16} + 4131u^{17} + 67267u^{18} + 236808u^{19} - 614784u^{20} - 12412763u^{21} + 2839656u^{22} + 414942978u^{23} - 2018275270u^{24} + 4793140380\tfrac{3}{5}u^{25} - 6835882485u^{26} + 6156900766u^{27} - 3449297064u^{28} + 1102444428u^{29} - 154094468\tfrac{7}{10}u^{30},$$

$$L_{11} = 24u^{16} + 660u^{17} + 6656u^{18} + 70275u^{19} + 602928u^{20} + 423644u^{21} - 12635748u^{22} - 86214999u^{23} + 306005260u^{24} + 2620578876u^{25} - 19491928200u^{26} + 59739201959u^{27} - 108143883564u^{28} + 126406988784u^{29} - 97076564452u^{30} + 47569139712u^{31} - 13540389348u^{32} + 1708597533\tfrac{1}{11}u^{33}.$$

Body-Centered Cubic

$$L_1 = u^4,$$

$$L_2 = 4u^7 - 4\tfrac{1}{2}u^8,$$

$$L_3 = 28u^{10} - 64u^{11} + 36\tfrac{1}{3}u^{12},$$

$$L_4 = 12u^{12} + 204u^{13} - 798u^{14} + 948u^{15} - 366\tfrac{1}{4}u^{16},$$

$$L_5 = 12u^{14} + 216u^{15} + 1262u^{16} - 9072u^{17} + 17592u^{18} - 14184u^{19} + 4174\tfrac{1}{5}u^{20},$$

$$L_6 = 27u^{16} + 312u^{17} + 2368u^{18} + 4312u^{19} - 92992u^{20} + 275021\tfrac{1}{3}u^{21} - 353640u^{22} + 216036u^{23} - 51444\tfrac{1}{2}u^{24},$$

$$L_7 = 72u^{18} + 704u^{19} + 4404u^{20} + 17616u^{21} - 36348u^{22} - 833064u^{23} + 3795726u^{24} - 7072736u^{25} + 6798900u^{26} - 3344712u^{27} + 669438\tfrac{1}{7}u^{28},$$

$$L_8 = 4u^{19} + 198u^{20} + 2016u^{21} + 10300u^{22} + 41352u^{23} + 55536u^{24} - 989076u^{25} - 6007194u^{26} + 46866408u^{27} - 122039509u^{28} + 166096620u^{29} - 127471458u^{30} + 52501716u^{31} - 9066913\tfrac{1}{8}u^{32},$$

$$L_9 = 24u^{21} + 692u^{22} + 5816u^{23} + 30714u^{24} + 99648u^{25} + 226692u^{26} - 887688u^{27} - 13103579u^{28} - 24522136u^{29} + 514861877\tfrac{1}{3}u^{30} - 1874111776u^{31} + 3435605052u^{32} - 3684304933\tfrac{1}{3}u^{33} + 2353070344u^{34} - 833603008u^{35} + 126632261\tfrac{1}{9}u^{36}.$$

APPENDIX IV. EXPANSIONS FOR ln Λ AND $I(u)$

Diamond

$$I(u) = 1 - 2u^2 - 8u^3 - 26u^4 - 80u^5 - 268u^6 - 944u^7 - 3474u^8 - 13072u^9 - 49672u^{10} - 191272u^{11} - 744500u^{12} + \cdots,$$

$$\ln \Lambda = u^2 + 2u^3 + 3\tfrac{1}{2}u^4 + 6u^5 + 12\tfrac{1}{3}u^6 + 30u^7 + 83\tfrac{3}{4}u^8 + 250\tfrac{2}{3}u^9 + 768\tfrac{1}{5}u^{10} + 2442u^{11} + 8009\tfrac{1}{6}u^{12} + \cdots.$$

Simple Cubic

$$I(u) = 1 - 2u^3 - 12u^5 + 14u^6 - 90u^7 + 192u^8 - 792u^9 + 2148u^{10} - 7716u^{11} + 23262u^{12} - 79512u^{13} + 252054u^{14} - 846628u^{15} + 2753520u^{16} - 9205800u^{17} + 30371124u^{18} + \cdots,$$

$$\ln \Lambda = u^3 + 3u^5 - 3\tfrac{1}{2}u^6 + 15u^7 - 33u^8 + 104\tfrac{1}{3}u^9 - 280\tfrac{1}{2}u^{10} + 849u^{11} - 2461\tfrac{3}{4}u^{12} + 7485u^{13} - 22534\tfrac{1}{2}u^{14} + 69393\tfrac{1}{5}u^{15} - 213754\tfrac{1}{2}u^{16} + 666750u^{17} - 2086734\tfrac{1}{6}u^{18} + \cdots.$$

Body-Centered Cubic

$$I(u) = 1 - 2u^4 - 16u^7 + 18u^8 - 168u^{10} + 384u^{11} - 314u^{12} - 1632u^{13} + 6264u^{14} - 9744u^{15} - 10014u^{16} + 86976u^{17} - 205344u^{18} + 80176u^{19} + 1009338u^{20} - 3579568u^{21} + 4575296u^{22} + 8301024u^{23} + \cdots,$$

$$\ln \Lambda = u^4 + 4u^7 - 4\tfrac{1}{2}u^8 + 28u^{10} - 64u^{11} + 48\tfrac{1}{3}u^{12} + 204u^{13} - 786u^{14} + 1164u^{15} + 922\tfrac{3}{4}u^{16} - 8760u^{17} + 20032u^{18} - 9164u^{19} - 84215\tfrac{4}{5}u^{20} + 294677\tfrac{1}{3}u^{21} - 378996u^{22} - 569704u^{23} + \cdots.$$

Face-Centered Cubic

$$I(u) = 1 - 2u^6 - 24u^{11} + 26u^{12} - 48u^{15} - 252u^{16} + 720u^{17} - 438u^{18} - 192u^{19} - 984u^{20} - 1008u^{21} + 12924u^{22} - 19536u^{23} + 3062u^{24} - 8280u^{25} + 26694u^{26} + 153536u^{27} - 507948u^{28} + \cdots,$$

$$\ln \Lambda = u^6 + 6u^{11} - 6\tfrac{1}{2}u^{12} + 8u^{15} + 42u^{16} - 120u^{17} + 72\tfrac{1}{3}u^{18} + 24u^{19} + 123u^{20} + 126u^{21} - 1623u^{22} + 2418u^{23} - 495\tfrac{1}{4}u^{24} + 822u^{25} - 2703u^{26} - 15512u^{27} + 50538u^{28} + \cdots.$$

APPENDIX V. ANTIFERROMAGNETIC EXPANSIONS FOR ln Λ^a AND THE LOW-TEMPERATURE SUSCEPTIBILITY

Honeycomb

$$2 \ln \Lambda^a = y^3(\theta_1) + y^4(3) + y^5(3\theta_1) + y^6(10 + \tfrac{1}{2}\theta_2) + y^7(12\theta_1) + y^8(43\tfrac{1}{2} + 6\theta_2) + y^9(68\theta_1 + 1\tfrac{1}{3}\theta_3) + y^{10}(252 + 55\tfrac{1}{2}\theta_2) + y^{11}(471\theta_1 + 24\theta_3) + y^{12}(1762 + 507\theta_2 + 4\tfrac{1}{4}\theta_4) + y^{13}(3696\theta_1 + 321\theta_3) + \cdots,$$

$$\chi^a(y) = 4y^3 + 12y^5 + 8y^6 + 48y^7 + 96y^8 + 320y^9 + 888y^{10} + 2748y^{11} + 8384y^{12} + 26340y^{13} + \cdots.$$

Simple Quadratic

$$2 \ln \Lambda^a = y^4(\theta_1) + y^6(4) + y^8(-2 + 6\theta_1 - \tfrac{1}{2}\theta_2) + y^{10}(32 - 8\theta_1 + 4\theta_2) + y^{12}(-54 + 75\theta_1 - 12\theta_2 + 1\tfrac{1}{3}\theta_3) + y^{14}(428 - 176\theta_1 + 100\theta_2 - 8\theta_3) + y^{16}(-1095 + 1284\theta_1 - 324\theta_2 + 80\theta_3 - 2\tfrac{1}{4}\theta_4) + y^{18}(7469\tfrac{1}{3} - 3836\theta_1 + 2388\theta_2 - 364\theta_3 + 36\theta_4) + \cdots,$$

$$\chi^a(y) = 4y^4 + 16y^8 + 32y^{10} + 156y^{12} + 608y^{14} + 2688y^{16} + 12064y^{18} + \cdots.$$

Diamond

$$2 \ln \Lambda^a = y^4(\theta_1) + y^6(4) + y^8(-4 + 6\theta_1 - \tfrac{1}{2}\theta_2) + y^{10}(36 - 16\theta_1 + 4\theta_2) + y^{12}(-130 + 100\theta_1 - 24\theta_2 + 1\tfrac{1}{3}\theta_3) + y^{14}(716 - 472\theta_1 + 160\theta_2 - 16\theta_3) + y^{16}(-3528 + 2656\theta_1 - 954\theta_2 + 150\theta_3 - 4\tfrac{1}{4}\theta_4) + y^{18}(19365\tfrac{1}{3} - 14328\theta_1 + 5984\theta_2 - 1164\theta_3 + 76\theta_4) + y^{20}(-105198 + 81866\theta_1 - 36330\theta_2 + 8675\theta_3 - 860\theta_4 + 16\tfrac{1}{5}\theta_5) + y^{22}(595860 - 467188\theta_1 + 225048\theta_2 - 61176\theta_3 + 8184\theta_4 - 356\theta_5) + y^{24}(-3402210\tfrac{1}{3} + 2735304\theta_1 - 1385980\theta_2 + 424900\theta_3 - 69928\theta_4 + 4882\theta_5 - 63\tfrac{2}{3}\theta_6) + \cdots,$$

$$\chi^a(y) = 4y^4 + 16y^8 + 64y^{12} + 96y^{14} + 488y^{16} + 1392y^{18} + 5064y^{20} + 17856y^{22} + 65576y^{24} + \cdots.$$

Simple Cubic

$$2 \ln \Lambda^a = y^6(\theta_1) + y^{10}(6) + y^{12}(-6 - \tfrac{1}{2}\theta_2) + y^{14}(15\theta_1) + y^{16}(6 - 36\theta_1) + y^{18}(126 + 21\theta_1 + 20\theta_2 + \tfrac{1}{3}\theta_3) + y^{20}(-477 + 48\theta_1 - 90\theta_2) + y^{22}(594 + 411\theta_1 + 126\theta_2 + 15\theta_3) + y^{24}(445 - 2676\theta_1 + 112\theta_2 - 120\theta_3 - \tfrac{1}{4}\theta_4) + y^{26}(2034 + 5595\theta_1 + 552\theta_2 + 315\theta_3 + 6\theta_4) + y^{28}(-27306 - 696\theta_1 - 8095\tfrac{1}{2}\theta_2 - 90\theta_4) + y^{30}(84120 + 256\theta_1 + 26740\theta_2 - 84\theta_3 + 420\theta_4 + 1\tfrac{1}{5}\theta_5) + y^{32}(-74361 - 137592\theta_1 - 24342\theta_2 - 14184\theta_3 - 420\theta_4 - 36\theta_5) + y^{34}(-50160 + 639267\theta_1 - 22356\theta_2 + 75780\theta_3 - 1176\theta_4 + 315\theta_5) + y^{36}(-1007677 - 1056396\theta_1 - 374891\tfrac{1}{2}\theta_2 - 137168\theta_3 - 13650\theta_4 - 784\theta_5 - 6\tfrac{1}{6}\theta_6) + \cdots.$$

$$\chi^a(y) = 4y^6 - 8y^{12} + 60y^{14} - 144y^{16} + 416y^{18} - 1248y^{20} + 4200y^{22} - 13248y^{24} + 42936y^{26} - 138072y^{28} + 452840y^{30} - 1480944y^{32} + 4883688y^{34} - 16114784y^{36} + \cdots.$$

Body-Centered Cubic

$$2 \ln \Lambda^a = y^8(\theta_1) + y^{14}(8) + y^{16}(-8 - \tfrac{1}{2}\theta_2) + y^{20}(28\theta_1) + y^{22}(-64\theta_1) + y^{24}(24 + 36\theta_1 + \tfrac{1}{3}\theta_3) + y^{26}(296 + 56\theta_2) + y^{28}(-1148 + 12\theta_1 - 224\theta_2) + y^{30}(1320 + 216\theta_1 + 288\theta_2) + y^{32}(-444 + 1192\theta_1 - 117\theta_2 + 70\theta_3 - \tfrac{1}{4}\theta_4) + y^{34}(432 - 8624\theta_1 + 96\theta_2 - 448\theta_3) + y^{36}(3224 + 16656\theta_1 + 756\theta_2 + 1008\theta_3) + y^{38}(4456 - 12544\theta_1 + 2032\theta_2 - 936\theta_3 + 56\theta_4) + y^{40}(-112700 + 7948\theta_1 - 35884\theta_2 + 630\theta_3 - 560\theta_4 + \tfrac{1}{5}\theta_5) + y^{42}(332602\tfrac{2}{3} + 16464\theta_1 + 108720\theta_2 + 1176\theta_3 + 2016\theta_4) + y^{44}(-402840 - 35824\theta_1 - 138644\theta_2 + 140\theta_3 - 3276\theta_4 + 28\theta_5) + y^{46}(295488 - 733168\theta_1 + 106776\theta_2 - 93632\theta_3 + 3024\theta_4 - 448\theta_5) + \cdots.$$

$$\chi^a(y) = 4y^8 - 8y^{16} + 112y^{20} - 256y^{22} + 156y^{24} + 896y^{26} - 3536y^{28} + 5472y^{30} + 5400y^{32} - 49088y^{34} + 115008y^{36} - 47776y^{38} - 555492y^{40} + 1976736y^{42} - 2563424y^{44} - 4446272y^{46} + \cdots.$$

Special Class of Feynman Integrals in Two-Dimensional Space–Time*

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Contributions of Feynman diagrams consisting of a single loop with an arbitrary number of vertices are explicitly evaluated in two-dimensional space–time. The result can be written as a sum of logarithms multiplied by algebraic expressions. Each logarithm is characteristic of a simple diagram of one loop with two external lines, while the coefficients can be obtained from rules analogous to the rules of residue calculus.

1. INTRODUCTION

ONE of the most useful calculational techniques in quantized field theory is the use of Feynman diagrams. Even if standard methods for the evaluation of such diagrams have been developed, mainly the introduction of so-called Feynman auxiliary variables of integration, no general method exists which allows one to calculate in detail and with ease the contribution from a given diagram with a large number of lines. The standard method gives rise to rather extensive integrations also in comparatively simple cases. In this paper we are going to study diagrams consisting of a single loop but with an arbitrary number of external lines. As is well known, such a diagram gives rise to an integral of the following form

$$F(z_{ik}, a_k) = \int \frac{d\mathbf{q}}{\prod_{k=0}^{n} [(q - p_k)^2 + a_k - i\epsilon]}, \tag{1}$$

$$z_{ik} = -(\mathbf{p}_i - \mathbf{p}_k)^2 = (p_{i0} - p_{k0})^2 - (\bar{\mathbf{p}}_i - \bar{\mathbf{p}}_k)^2. \tag{1a}$$

Here, the differences of the vectors $\mathbf{p}_j$ $(j=0, 1, \cdots, n)$ are the external energy momentum vectors of the diagram and the a_j denote the squares of the masses of the particles corresponding to the internal lines of the polygon. We are interested in the function $F(z_{ik}, a_k)$ considered as an analytic function of the squares z_{ik} of all the differences of the vectors $\mathbf{p}_k$ and as a function of the internal masses a_k. The latter quantities may be real or complex. In general, this analytic function has a complicated Riemann surface with many branch points. We define the principal (or physical) sheet of the Riemann surface as the sheet obtained when all vectors and masses in Eq. (1) are real and the singularities in the integrand are interpreted with the aid of the conventional $i\epsilon$ indicated explicitly in Eq. (1) and corresponding to the usual time-ordered product. The integral is supposed to be evaluated for this case and the result analytically continued from there.

The standard technique for the evaluation of (1) is to use the identity[1]

$$(A_0 A_1 \cdots A_n)^{-1} = n! \int_0^1 \cdots \int_0^1 d^{n+1}\alpha \times \delta(1 - \sum \alpha_k)(\sum A_k \alpha_k)^{-n-1}, \tag{2}$$

to write the integral in Eq. (1) as follows

$$F(z_{ik}, a_k) = n! \int \cdots \int d^{n+1}\alpha\ \delta(1 - \sum \alpha_k) \int \frac{dq}{D^{n+1}}, \tag{3}$$

$$D = q^2 - 2\sum \mathbf{q}\mathbf{p}_k \alpha_k + \sum (\mathbf{p}_k^2 + a_k)\alpha_k - i\epsilon. \tag{3a}$$

A simple translation of the variable of integration $\mathbf{q}$ allows us to write the expression (3) in the form

$$F(z_{ik}, a_k) = n! \int \cdots \int d^{n+1}\alpha \times \delta(1 - \sum \alpha_k) \int \frac{d\mathbf{q}}{(\mathbf{q}^2 + A - i\epsilon)^{n+1}}, \tag{4}$$

$$A = \sum (\mathbf{p}_k^2 + a_k)\alpha_k - (\sum \mathbf{p}_k \alpha_k)^2 = \sum_{j<k} (\mathbf{p}_j - \mathbf{p}_k)^2 \alpha_j \alpha_k + \sum a_k \alpha_k = \sum a_k \alpha_k - \sum_{j<k} z_{jk} \alpha_j \alpha_k. \tag{4a}$$

The integration over the vector $\mathbf{q}$ can now be performed. If we assume that we are working in a space with one time dimension and $m - 1$ space dimensions (an m-dimensional Lorentz space) we find

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[1] R. P. Feynman, Phys. Rev. 76, 785 (1949).

$$\int \frac{d^m\mathbf{q}}{(\mathbf{q}^2 + A - i\epsilon)^{n+1}} = \frac{C_n^{(m)}}{n!\, A^{n+1-\frac{1}{2}m}}; \qquad n + 1 - \tfrac{1}{2}m > 0, \tag{5}$$

$$C_n^{(m)} = i\pi^{\frac{1}{2}m}\Gamma(n + 1 - \tfrac{1}{2}m). \tag{5a}$$

If the value of n is not larger than $\frac{1}{2}m - 1$, the integral diverges and the function $F(z_{jk}, a_k)$ is not well defined. In the opposite case we get by combining Eqs. (4) and (5)

$$F(z_{jk}, a_k) = C_n^{(m)} \int \cdots \int d^{n+1}\alpha \times \delta(1 - \sum \alpha_k) A^{-n-1+\frac{1}{2}m}. \tag{6}$$

This is the standard expression for the function F. The explicit evaluation of this quantity requires that all the integrations over α_k are performed. This is a time-consuming task especially if n is large.

In the particular case $n + 1 = m = 2$ we find directly from Eq. (6)

$$F(z_{12}, a_1, a_2) = i \iint \frac{d\alpha_1\, d\alpha_2\, \delta(1 - \alpha_1 - \alpha_2)}{a_1\alpha_1 + a_2\alpha_2 - z_{12}\alpha_1\alpha_2} = \frac{i\pi}{R_{12}^{\frac{1}{2}}} \log X_{12}, \tag{7}$$

$$R_{12} \equiv \lambda(z_{12}, a_1, a_2) = (z_{12} - a_1 - a_2)^2 - 4a_1a_2, \tag{7a}$$

$$X_{12} = \frac{z_{12} - a_1 - a_2 - R_{12}^{\frac{1}{2}}}{z_{12} - a_1 - a_2 + R_{12}^{\frac{1}{2}}}. \tag{7b}$$

This function is so important in what follows that we introduce a special notation for it and denote it by $L_{12} \equiv L(z_{12}, a_1, a_2)$. It is the simplest possible case of a function obtainable from a Feynman diagram and corresponds to a diagram with two external lines and a simple "bubble" of internal lines between the two vertices.

The integral in Eq. (7) is supposed to be evaluated, e.g., for z_{12} negative and real and the quantities a_1 and a_2 positive and real. In that case the denominator never vanishes in the interval of integration and $-iL_{12}$ is a positive real number. Consequently, the logarithm is to be taken on its principal sheet for this case. The square root is, e.g., defined to have a positive real part. This definition makes the number X_{12} real and larger than one for the case just considered. The function L_{12} is defined for other values of z_{12} or/and a_1 and a_2 by analytic continuation from the domain just mentioned. As an example we mention that when a_1 and a_2 are positive and real, the representation

$$L(z, a, b) = 2i\pi \int_{M^2}^{\infty} \frac{du}{[\lambda(u, a, b)]^{\frac{1}{2}}} \frac{1}{u - z}, \tag{8}$$

$$M^2 = (a^{\frac{1}{2}} + b^{\frac{1}{2}})^2, \tag{8a}$$

explicitly shows that L_{12} is an analytic function of z regular in the whole complex plane except for a cut along the positive real axis above M^2.

The main result to be proved below is that every function of the type indicated in Eq. (1) and with $m = 2$ can be written as a sum of terms L_{ij} defined in Eq. (7) with coefficients which can be written down by inspection. The practical usefulness of the result is presumably not very great as diagrams in two-dimensional space–time are not of immediate physical interest. However, field theories in two-dimensional space time are occasionally used as models because of the simplifications obtained when the dimensionality of space is decreased[2] and our result may be of interest in such cases. Actually, the result presented here was found during an investigation of the analytic properties of certain perturbation theory three-point functions. In this case it can be shown that it is enough to study the diagram in question in two-dimensional Lorentz space, so these reduction formulas proved quite useful in problems of actual physical interest. There are also indications that generalizations of our result to higher dimensions are possible even if the formulas become more complicated when the number of dimensions is increased.[3]

2. A SPECIAL INTEGRATION TECHNIQUE IN TWO-DIMENSIONAL SPACE-TIME

An explicit evaluation of the α integrals in Eq. (6) is time consuming for large values of n even in the case $m = 2$. In principle, it also appears to be a somewhat round-about way to evaluate the two-dimensional integral in Eq. (1) in terms of the n-dimensional integral in Eq. (6). The purpose of the representation (2), when originally introduced, was to diminish the number of integrations and not to increase them. This goal is not achieved unless we also have $n < m$. In this section we want to develop another technique for the evaluation of the integral (1) taking explicit advantage of the simplifications obtained for $m = 2$. For this purpose we introduce "light cone coordinates" q_+, q_- for

[2] Compare from, e.g., W. E. Thirring, Ann. Phys. (N.Y.) **3**, 91 (1958).

[3] We mention in this connection the papers by F. R. Halpern, Phys. Rev. Letters **10**, 310 (1963) and L. M. Brown, Nuovo Cimento **22**, 178 (1961). Brown indicates how the general diagram of one loop with n vertices ($n \geq 6$) can be reduced in principal to the "pentagon" with five vertices; Halpern then shows how to reduce the "pentagon" to a "square" with four vertices. However, it is not known whether the generalization to higher dimensions of the formula for the coefficients in the two-dimensional case given in Eq. (25) below is sufficiently simple to be useful.

the vector q by the definition

$$q_s = q_0 + q_x, \tag{9a}$$

$$q_t = q_0 - q_x, \tag{9b}$$

and analogous definitions for all other vectors. In terms of these variables we have, e.g.,

$$q^2 = -q_s q_t, \tag{10a}$$

$$dq = dq_0 dq_x = \tfrac{1}{2} dq_s dq_t, \tag{10b}$$

$$2pq = -(p_s q_t + p_t q_s). \tag{10c}$$

Further, the integral (1) can now be written as follows

$$F(z_{jk}, a_k) = \tfrac{1}{2} \iint \frac{dq_s\, dq_t}{\prod [a_k - (q_s - p_{k,s})(q_t - p_{k,t}) - i\epsilon]}. \tag{11}$$

Concentrating our attention, e.g., on the integration over q_s we note that the integrand is an analytic function of q_s with simple poles at the points

$$q_s^j = p_{j,s} + (a_j - i\epsilon)/(q_t - p_{j,t}); \quad j = 0, 1, \cdots, n. \tag{12}$$

For $n \geq 1$ the integrand vanishes at infinity so rapidly that the contribution to the integral from a large circle vanishes in the limit when the radius of the circle goes to infinity. Closing the path of integration in the lower half-plane, we can write the function F in Eq. (11) as a sum of residues as follows

$$F(z_{jk}, a_k) = i\pi \sum_j \int dq_t (q_t - p_{j,t})^{n-1} \times \theta(q_t - p_{j,t}) D_j^{-1}, \tag{13}$$

$$D_j = \prod_{k \neq j} [(a_j - i\epsilon)(p_{k,t} - q_t) - (a_k - i\epsilon)(p_{j,t} - q_t) - (p_{j,s} - p_{k,s})(q_t - p_{j,t})(q_t - p_{k,t})]. \tag{13a}$$

An immediate consequence of the result (13) is that the whole function $F(z_{jk}, a_k)$ can be written as a sum of terms each of which is not more complicated than a logarithm. This fact is not evident from the representation (6).

The algebraic structure of the result (13) appears to be rather complicated, especially as we have to make a partial fractions expansion in terms of the variable q_t to perform the remaining integrations. However, the main contribution to the partial fractions expansion just mentioned comes from the product of all factors except one in (13a) evaluated at a value of q_t which makes the remaining factor equal to zero. Each factor in (13a) is given by one of the original denominators in (1) multiplied by $q_t - p_{j,t}$ and should be evaluated at a value of q_s which makes the jth denominator in (1) vanish. Further, each factor in (13a) is of the second order in q_t and it follows that there are two values of the vector q which make two of the original denominators in (1) equal to zero at the same time. Let us denote the two vectors q which makes the kth and jth denominators in the original integrand simultaneously equal to zero by $q_{jk}^{(\sigma)}$; $\sigma = 1, 2$. Using this notation we can write the partial fractions expansion of (13) in the following form

$$F(z_{jk}, a_k) = i\pi \sum_j dq_t \sum_{k \neq j} \sum_\sigma A_{jk}^{(\sigma)} [(p_{k,s} - p_{j,s}) \times (q_{jk}^{(\sigma)} - q_{jk}^{(\sigma')})]^{-1} \frac{\theta(q_t - p_{j,t})}{q_t - q_{jk,t}^{(\sigma)}}; \quad \sigma \neq \sigma', \tag{14}$$

$$[A_{jk}^{(\sigma)}]^{-1} = \prod_{l \neq j,k} [(q_{jk}^{(\sigma)} - p_l)^2 + a_l]. \tag{14a}$$

Noting that the same coefficient $A_{jk}^{(\sigma)}$ appears twice in the sum in Eq. (14) we can collect the terms in this expression in the following way

$$F(z_{jk}, a_k) = i\pi \sum_{j<k} \sum_\sigma A_{jk}^{(\sigma)} f_{jk}^{(\sigma)}, \tag{15}$$

$$f_{jk}^{(\sigma)} = \int dq_t (p_{k,s} - p_{j,s})^{-1} (q_{jk,t}^{(\sigma)} - q_{jk,t}^{(\sigma')})^{-1} \times (q_t - q_{jk,t}^{(\sigma)})^{-1} [\theta(q_t - p_{j,t}) - \theta(q_t - p_{k,t})]. \tag{15a}$$

The domain of integration in Eq. (15a) is effectively a finite piece of the real axis and one finds

$$f_{jk}^{(\sigma)} = (p_{k,s} - p_{j,s})^{-1} (q_{jk,t}^{(\sigma)} - q_{jk,t}^{(\sigma')})^{-1} \log \frac{p_{k,t} - q_{jk,t}^{(\sigma)}}{p_{j,t} - q_{jk,t}^{(\sigma)}}. \tag{16}$$

Equations (15) and (16) give, in principle, a complete answer for the Feynman integral (1) in two space–time dimensions.

3. ALGEBRAIC SIMPLIFICATIONS OF THE RESULT

The formulas obtained in the previous section appear somewhat forbidding. However, the general structure is not too complicated and easily seen though once the significance of the vectors $q_{jk}^{(\sigma)}$ is realized. For an explicit evaluation of both the expressions $A_{jk}^{(\sigma)}$ in Eq. (14a) and $f_{jk}^{(\sigma)}$ in Eq. (16) it is desirable to have formulas for the vectors $q_{jk}^{(\sigma)}$. To achieve this we have to solve the equations

$$(q - p_j)^2 + a_j = 0, \tag{17a}$$

$$(q - p_k)^2 + a_k = 0. \tag{17b}$$

Let us denote the vector $q - p_j$ by Q for a moment.

The two Eqs. (17) then take the form

$$Q^2 + a_j = 0, \tag{18a}$$

$$2Qp_{jk} - a_j + p_{jk}^2 + a_k = 0, \tag{18b}$$

$$p_{jk} = p_j - p_k. \tag{18c}$$

Consequently, the vector Q has a given length and a given projection on the vector p_{jk}. In two-dimensional space–time there are just two such vectors viz.

$$Q = (2p_{jk}^2)^{-1}[(p_{jk}^2 + a_k - a_j)p_{kj} \pm \hat{p}_{kj}(\lambda(-p_{kj}^2, a_j, a_k))^{\frac{1}{2}}]$$

$$= \frac{1}{2z_{jk}}[(z_{jk} + a_j - a_k)p_{kj} \pm \hat{p}_{kj}R_{jk}^{\frac{1}{2}}]. \tag{19}$$

The vector $\hat{p}_{jk}$ in Eq. (19) is a vector orthogonal to p_{jk}. To be precise, we can define

$$p = (p_x, p_0), \tag{20a}$$

$$\hat{p} = (p_0, p_x), \tag{20b}$$

$$\hat{p}^2 = -p^2. \tag{20c}$$

Substituting back in the equations above, we find that the vector q in Eq. (17) is given by

$$q_{jk}^{(\sigma)} = \frac{1}{2}\left[p_j + p_k + \frac{a_j - a_k}{z_{jk}}(p_k - p_j) \pm (\hat{p}_k - \hat{p}_j)\frac{R_{jk}^{\frac{1}{2}}}{z_{jk}}\right]. \tag{21}$$

The conventions we have introduced in Eq. (15) are such that $q_{jk}^{(\sigma)}$ is symmetric in j and k. We can make this prescription precise by defining the sign in Eq. (21) to be $+1$ for $\sigma = 1$ and $j < k$. In this way we find

$$(p_{k,s} - p_{j,s})(q_{jk,t}^{(\sigma)} - q_{jk,t}^{(\sigma')}) = (-1)^{\sigma}R_{jk}^{\frac{1}{2}}; \quad j < k, \tag{22a}$$

$$\frac{p_{k,t} - q_{jk,t}^{(\sigma)}}{p_{j,t} - q_{jk,t}^{(\sigma)}} = \frac{-1}{2a_j}[z_{jk} - a_k - a_j - (-1)^{\sigma}R_{jk}^{\frac{1}{2}}]; \quad j < k. \tag{22b}$$

Equations (22) allow us to simplify Eq. (16) in the following way

$$f_{jk}^{(\sigma)} = \frac{(-1)^{\sigma}}{R_{jk}^{\frac{1}{2}}}\log\frac{z_{jk} - a_k - a_j - (-1)^{\sigma}R_{jk}^{\frac{1}{2}}}{-2a_j}. \tag{23}$$

The expression given in Eq. (15) can now be further simplified by noting that the coefficients in the partial fractions expansion (14) must fulfil the sum rule

$$\sum_k \sum_{\sigma} \frac{(-1)^{\sigma}}{R_{jk}^{\frac{1}{2}}} A_{jk}^{(\sigma)} = 0 \quad \text{for all } j. \tag{24}$$

Equation (24) allows us to write Eq. (15) in the following remarkably simple form

$$F(z_{jk}, a_k) = \frac{i\pi}{2}\sum_{j<k}[A_{jk}^{(1)} + A_{jk}^{(2)}]\frac{1}{R_{jk}^{\frac{1}{2}}} \times \log\frac{z_{jk} - a_k - a_j - R_{jk}^{\frac{1}{2}}}{z_{jk} - a_k - a_j + R_{jk}^{\frac{1}{2}}}$$

$$= \sum_{j<k} \tfrac{1}{2}(A_{jk}^{(1)} + A_{jk}^{(2)})L_{jk}. \tag{25}$$

4. GENERALIZATION TO MULTINOMIAL NUMERATORS

In many problems, such as those involving particles with nonzero spin, integrals more general than F in Eq. (1) appear. They are of the form

$$F(z_{jk}, a_k) = \int \frac{dqN(p, q)}{\prod_{k=0}^{n}[(q - p_k)^2 + a_k - i\epsilon]}, \tag{26}$$

where the new factor N is any multinomial of the components of the p_j's and q, such that the integral is still convergent. We now want to show that also in this case one obtains a result in the form of Eq. (25) where the $A_{jk}^{(\sigma)}$ now include the factor $N(p, q_{jk}^{(\sigma)})$.

The proof of this result could be made by the integration technique of Sec. 2, but we find it easier to use another approach and to proceed by induction. Let us assume that the proof has been done for all multinomials of a given degree in the components of q and for all n. An additional factor q can be introduced into the numerator by inserting another factor $(b^2/2)[(q - Q)^2 + b - i\epsilon]^{-1}$ in the integrand, differentiating with respect to Q, and then taking the limit when $b \to \infty$ and $Q \to 0$. The result is

$$\int \frac{dqN(p, q)q}{\prod[(q - p_k)^2 + a_k - i\epsilon]} = F_1 + F_2, \tag{27}$$

where

$$F_1 = \tfrac{1}{4}\lim_{\substack{b\to\infty \\ Q\to 0}} \nabla_Q \sum_{j<k}\sum_{\sigma} A_{jk}^{(\sigma)} \frac{b^2}{(q_{jk}^{(\sigma)} - Q)^2 + b} L_{jk}$$

$$= \tfrac{1}{2}\sum_{j<k}\sum_{\sigma} A_{jk}^{(\sigma)} q_{jk}^{(\sigma)} L_{jk}, \tag{27a}$$

and

$$A_{jk}^{(\sigma)} = N(p, q_{jk}^{(\sigma)}) \prod_{l\neq j,k}[(q_{jk}^{(\sigma)} - p_l)^2 + a_l]^{-1}. \tag{27b}$$

The second term in Eq. (27) is given by

$$F_2 = \tfrac{1}{4}\lim_{\substack{b\to\infty \\ Q\to 0}} \nabla_Q \sum_k \frac{b^2 N(p, q_k^{(\sigma)})}{\prod_{i\neq k}[(q_k^{(\sigma)} - p_i)^2 + a_i]} \times L(-(p_k - Q)^2, b, a_k), \tag{28a}$$

where $q_k^{(\sigma)}$ for $\sigma = 1, 2$ are the two solutions of

$$(q_k^{(\sigma)} - Q)^2 + b = 0, \qquad (q_k^{(\sigma)} - p_k)^2 + a_k = 0. \tag{28b}$$

We note from Eq. (27a) that F_1 is the desired result for the numerator $N(p, q)q$ needed for the induction proof. Therefore, we must only show that F_2 vanishes. From Eqs. (28b), using the solution (21), we find that each component of both of the vectors $q_k^{(\sigma)}$ as well as the $(q_k^{(\sigma)})^2$, are of the first order in b when $b \to \infty$. An elementary estimate then shows that, if the integral in Eq. (27) is convergent, the term F_2 vanishes at least as rapidly as $b^{-1} \log b$. This completes the proof.

5. DISCUSSION

The result just obtained can be summarized in the following way.

The contribution of the Feynman diagram (1) or (26) in two-dimensional space–time can be written as a sum of terms where each term is obtained by applying rules:

(i) Pick out all possible pairs of denominators $(q - p_i)^2 + a_i$ and $(q - p_k)^2 + a_k$ in (1) and find the two vectors $q_{ik}^{(\sigma)}$ which make both these denominators equal to zero. An explicit formula for these vectors is given by Eq. (21).

(ii) Substitute $q_{ik}^{(\sigma)}$ in all of the remaining factors in (1) or (26). This quantity is denoted by $A_{ik}^{(\sigma)}$.

(iii) Take the average of $A_{ik}^{(\sigma)}$ for the two possible values of σ.

(iv) Multiply by the function L_{ik} defined in Eqs. (7) and (8) and corresponding to a simple "bubble" with $p_i - p_k$ as external vector.

(v) Sum over all $j < k$.

In passing, we mention that a special case of Eq. (25) with $n = 3$ and corresponding to a "triangle" diagram has been noticed before.[4]

The possibility of generalizing our result to higher dimensions has already been mentioned.[3] Another generalization to be investigated is concerned with diagrams in two-dimensional space–time but of more complicated structure involving two or more closed loops. Even if we have no definite results to report for such cases we want to remark that the result (25) together with the representation (8) for the functions L_{ij} may be useful also in such cases. By performing one of the integrations with the aid of (25) and representing all the logarithms in the form (8) one brings the function in a shape where the second integration can again be performed with the aid of (25). Proceeding in this way it is possible to write the function of such a Feynman diagram in terms of a ν-fold integral, where ν is the number of closed loops in the diagram and not the number of internal lines. In certain cases, this might be a convenient intermediate step in the evaluation of the integral.

[4] G. Källén, A. Wightman, Dan. Mat. Fys. Skr. 1, No. 6 (1958). Cf. also Ref. 3.

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Exact Solution of a Many-Fermion System and Its Associated Boson Field

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Luttinger's exactly soluble model of a one-dimensional many-fermion system is discussed. We show that he did not solve his model properly because of the paradoxical fact that the density operator commutators $[\rho(p), \rho(-p')]$, which always vanish for any finite number of particles, no longer vanish in the field-theoretic limit of a filled Dirac sea. In fact the operators $\rho(p)$ *define* a boson field which is *ipso facto* associated with the Fermi–Dirac field. We then use this observation to solve the model, and obtain the exact (and now nontrivial) spectrum, free energy, and dielectric constant. This we also extend to more realistic interactions in an Appendix. We calculate the Fermi surface parameter $\tilde{n}_k$, and find: $\partial\tilde{n}_k/\partial k|_{k_F} = \infty$ (i.e., there exists a sharp Fermi surface) only in the case of a sufficiently weak interaction.

I. INTRODUCTION

THE search for a soluble but realistic model in the many-electron problem has been just about as unfruitful as the historic quest for the philosopher's stone, but has equally resulted in valuable byproducts. For example, 15 years ago Tomonaga[1] published a theory of interacting fermions which was soluble only in one dimension with the provision that certain truncations and approximations were introduced into his operators. Nevertheless he had success in showing approximate boson-like behavior of certain collective excitations, which he identified as "phonons." (Today we would denote these as "plasmons," following the work of Bohm and Pines.[2]) Lately, Luttinger[3] has revived interest in the subject by publishing a variant model of spinless and massless one-dimensional interacting fermions, which demonstrated a singularity at the Fermi surface, compatible with the results of the modern many-body perturbation theory.[4]

Unfortunately, in calculating the energies and wavefunctions of his model Hamiltonian, Luttinger fell prey to a subtle paradox inherent in quantum field theory[5] and *therefore did not achieve a correct solution of the problem he himself had posed.* In the present paper we shall give the solution to his interesting problem and calculate the free energy. We shall show the existence of collective plasmon modes, and shall calculate the singularity at the Fermi surface (which may in fact disappear if the interaction is strong enough), the energy of the plasmons, and the (nontrivial) dielectric constant of the system. In an Appendix we shall show how the model may be generalized in such a manner as to remove certain restrictions on the interactions which Luttinger had found necessary to impose.

It is fortunate that solid-state and many-body theorists have so far been spared the plagues of quantum field theory. Second quantization has been often just a convenient bookkeeping arrangement to save us from writing out large determinantal wavefunctions. However there is a difference between very large determinants and *infinitely* large ones; we shall show that one of the important differences *is the failure of certain commutators to vanish* in the field-theoretic limit when common sense and experience based on finite N tells us they *should* vanish! (Here N refers to the number of particles in the field.)

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[1] S. Tomonaga, Progr. Theoret. Phys. (Kyoto) 5, 544 (1950).

[2] D. Bohm and D. Pines, Phys. Rev. 92, 609 (1953).

[3] J. M. Luttinger, J. Math. Phys. 4, 1154 (1963). Note that we set his $v_0 = 1$, thereby fixing the unit of energy. References to this paper will be frequent, and will be denoted by L (72), for example, signifying his Eq. (72).

[4] J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960).

[5] Luttinger made a transformation, L (8), which was canonical in appearance only. But in the language of G. Barton [*Introduction to Advanced Field Theory*, (Interscience Publishers, Inc., New York, 1963), pp. 126 *et seq.*] this transformation connected two "unitarily inequivalent" Hilbert spaces, which has as a consequence that commutators, among other operators, must be reworked so as to be well-ordered in fermion field operators. It was first observed by Julian Schwinger [Phys. Rev. Letters 3, 296 (1959)] that the very fact that one postulates the existence of a ground state (i.e., the filled Fermi sea) *forces* certain commutators to be nonvanishing even though in first quantization they automatically vanish. The "paradoxical contradictions" of which Schwinger speaks seem to anticipate the difficulties in the Luttinger model.

We shall show that these nonvanishing commutators *define* boson fields which must *ipso facto* always be associated with a Fermi–Dirac field, and we shall use the ensuing commutation relations to solve Luttinger's model exactly. Because this model is soluble both in the Hilbert space of finite N and also in the Hilbert space $N = \infty$, with different physical behavior in each, we believe it has applications to the *theory of fields* which go beyond the study of the many-electron problem. The model can be extended to the case of electrons with spin. This has interesting consequences in the band *theory of ferromagnetism*, as will be discussed in some detail in an article under preparation.[5a]

II. MODEL HAMILTONIAN

We recall Luttinger's Hamiltonian[3] and recapitulate some of his results:

$$H = H_0 + H', \tag{2.1}$$

where the "unperturbed" part is

$$H_0 = \int_0^L dx\ \psi^+(x)\sigma_3 p\psi(x) \tag{2.2a}$$

$$= \sum_k (a_{1k}^* a_{1k} - a_{2k}^* a_{2k})k, \tag{2.2b}$$

and the interaction is

$$H' = 2\lambda \iint_0^L dx\ dy\ \psi_1^+(x)\psi_1(x) \times V(x-y)\psi_2^+(y)\psi_2(y) \tag{2.3a}$$

$$= \frac{2\lambda}{L} \sum \delta_{k_1+k_3,k_2+k_4} v(k_3 - k_4) \times a_{1k_1}^* a_{1k_2} a_{2k_3}^* a_{2k_4}. \tag{2.3b}$$

Here ψ is a two-component field and the form (b) of the operator is obtained from (a) by setting

$$\psi = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \begin{pmatrix} a_{1k} \\ a_{2k} \end{pmatrix}$$

and

$$\psi^+ = \frac{1}{\sqrt{L}} \sum_k e^{-ikx}(a_{1k}^*,\ a_{2k}^*), \tag{2.4}$$

with a_{ik}'s defined to be anticommuting fermion operators which obey the usual relations

$$\begin{aligned} &a_{ik}a_{i'k'} + a_{i'k'}a_{ik} \equiv \{a_{ik},\ a_{i'k'}\} = 0 \\ &\{a_{i,k}^*,\ a_{i'k'}^*\} = 0, \text{ and } \{a_{ik},\ a_{i'k'}^*\} = \delta_{ii'}\delta_{kk'}. \end{aligned} \tag{2.5}$$

Luttinger noted that for an appropriate operator S_0, the canonical transformation

$$\tilde{H} = e^{i\lambda S_0} H e^{-i\lambda S_0} \tag{2.6}$$

gave the result that

$$\tilde{H} = H_0, \tag{2.7}$$

and consequently that *the spectrum of* $H = H_0 + H'$ *was the same as that of* H_0, *independent of the interaction* $V(x-y)$. This can be explicitly verified for his choice of

$$S_0 = \iint_0^L dx\ dy\ \psi_1^+(x)\psi_1(x)E(x-y)\psi_2^+(y)\psi_2(y), \tag{2.8}$$

where $E(x)$, not to be confused with the energy E, is defined by:

$$\partial E(x-y)/\partial x \equiv V(x-y), \tag{2.9}$$

assuming that

$$\bar{V} \equiv \frac{1}{L}\int_0^L V(x)\,dx = 0. \tag{2.10}$$

In the Appendix we shall show among other things how to generalize to $\bar{V} \neq 0$. It is also simple and instructive to verify Eqs. (2.6) and (2.7) somewhat differently by using the *first* quantization,

$$H_0 = -i\sum_{n=1}^N \frac{\partial}{\partial x_n} + i\sum_{m=1}^M \frac{\partial}{\partial y_m} \tag{2.11}$$

and

$$H' = 2\lambda \sum_{n=1}^N \sum_{m=1}^M V(x_n - y_m), \tag{2.12}$$

where N and M are, respectively, the total number of "1" particles and "2" particles, with coordinates x_n and y_m, respectively. The properly antisymmetrized wavefunctions are given by

$$\Psi = \det|e^{ik_i x_j}| \det|e^{iq_i y_j}| \times \exp\left\{\sum_{n=1}^N \sum_{m=1}^M i\,E(x_n - y_m)\right\}. \tag{2.13}$$

Using Eqs. (2.9) and (2.10), Ψ is readily seen to obey Schrödinger's equation

$$H\Psi = E\Psi \tag{2.14}$$

with just the unperturbed eigenvalue

$$E = \sum_{n=1}^N k_n - \sum_{m=1}^M q_m. \tag{2.15}$$

The wavenumbers are of the form

$$k_i \quad \text{or} \quad q_j = 2\pi \text{ integer}/L, \tag{2.16}$$

as required for periodic boundary conditions. This is in exact agreement with the results of Ref. 3, and can also be checked in perturbation theory; first-

[5a] D. Mattis, Physics 1, 184 (1964).

order perturbation theory also gives vanishing results, and indeed, it is easy to verify that to every order in λ the cancellation is complete, in accordance with the exact result given above.

Up to this point, Luttinger's analysis (which we have briefly summarized) is perfectly correct. It is the next step that leads to difficulty. The Hamiltonian discussed so far has no ground-state energy; in order to remove this obstacle, and thereby establish contact with a real electron gas, Luttinger proposed modifying the model by "filling the infinite sea" of negative energy levels (i.e., all states with $k_1 <$ and $q_2 > 0$). Following L(8) we define b's and c's obeying the usual anticommutators, such that

$$a_{1k} = \begin{cases} b_k & k \geq 0 \\ c^*{}_k & k < 0, \end{cases} \qquad (2.17)$$

and

$$a_{2k} = \begin{cases} b_k & k < 0 \\ c_k^* & k \geq 0. \end{cases}$$

Using this notation the total particle-number operator becomes

$$\mathfrak{N} = \sum_{\text{all } k} b_k^+ b_k - c_k^+ c_k \qquad (2.17a)$$

(i.e., the number of particles minus the number of holes).

Since the Hamiltonian commutes with $\mathfrak{N}$ we can demand that $\mathfrak{N}$ have eigenvalue N_0. In the noninteracting ground state there are no holes and the b particles are filled from $-k_F$ to k_F where $k_F = \pi(N_0/L) = \pi\rho$. The noninteracting ground-state energy is $N_0\pi\rho +$ energy of the filled sea (W).

The kinetic energy assumes the form

$$H_0 = \sum_{\text{all } k} (b_k^* b_k + c_k^* c_k)\,|k| + W, \qquad (2.18)$$

where

$$W = \Big(\sum_{k<0} k - \sum_{k>0} k\Big) \qquad (2.18a)$$

is the infinite energy of the filled sea, an uninteresting c number which we drop henceforth in accordance with Luttinger's prescription. The interaction [H', Eq. (2.3) and the operator S_0, Eq. (2.8)] can also be expressed in the new language by means of the substitution (2.17). The reader will no doubt be surprised, as indeed we were, to find that now with the new operators, *Eq.* (2.7), *with* $\tilde{H}$ *defined in* (2.6), *is no longer obeyed.*

Upon further reflection one sees that this must be so, on the basis of very general arguments. In the new Hilbert space defined by the transformation to the particle–hole language (2.17), H is no longer unbounded from below and now has a ground state. A general and inescapable *concavity theorem* states that if $E_0(\lambda)$ is the ground-state energy in the presence of interactions, (2.3), then

$$\partial^2 E_0(\lambda)/\partial\lambda^2 < 0. \qquad (2.19)$$

This inequality is incompatible with the previous result, viz. all E = independent of λ, which was possible only in the strange case of a system without a ground state.

The same thing can be seen more trivially using second-order perturbation theory (first-order perturbation theory vanishes). It is easily seen that

$$E_0^{(2)} = -\Big(\frac{2\lambda}{L}\Big)^2 \sum_k \frac{|v(k)|^2}{2k} n_1(k) n_2(-k), \qquad (2.20)$$

where $n_1(k)$ and $n_2(k)$ are the number of ways of shifting a particle of type "1" and type "2" respectively by an amount k to an unoccupied state. A simple geometric exercise will convince the reader of the following facts: (1) if we start with a state having a finite number of particles, then n_1 and n_2 are *always* even functions of k (i.e., there are just as many ways to increase the momentum by k as to decrease it by the same amount.) (2) If we start with a filled infinite sea then there is no way to decrease the momentum of the "1" particles nor to increase the momentum of "2" particles. Hence for this second case $n_1(k)n_2(-k)$ is nonzero only for $k > 0$. Thus $E_0^{(2)}$ vanishes for a state with a finite number of particles, but it is negative for a filled sea.

If the reader is unconvinced by perturbation theory, then he can easily prove that E_0 is lowered by doing a variational calculation.

What has gone wrong? We turn to some algebra to resolve this paradox, and following this, present a solution of the field-theoretic problem defined by $H_0 + H'$ in the representation of b's and c's.

III. CASE OF THE FILLED DIRAC SEA

The various relevant operators are given below; the form (a) of each equation will *not* be used in the bulk of the paper, and is just given here for completeness. In the following equations, $p > 0$.

$$\rho_1(+p) \equiv \sum_k a_{1\,k+p}^* a_{1\,k} \qquad (3.1a)$$

$$= \sum_{k<-p} c_{k+p} c_k^* + \sum_{-p\leq k<0} b_{k+p}^* c_k^* + \sum_{k\geq 0} b_{k+p}^* b_k, \qquad (3.1b)$$

$$\rho_1(-p) \equiv \sum_k a_{1\,k}^* a_{1\,k+p} \qquad (3.2a)$$

$$= \sum_{k<-p} c_k c_{k+p}^* + \sum_{-p\leq k<0} c_k b_{k+p} + \sum_{k\geq 0} b_k^* b_{k+p}, \qquad (3.2b)$$

$$\rho_2(+p) \equiv \sum_k a^*_{2\,k+p} a_{2\,k} \tag{3.3a}$$

$$= \sum_{k<-p} b^*_{k+p} b_k + \sum_{-p\le k<0} c_{k+p} b_k + \sum_{k\ge 0} c_{k+p} c^*_k, \tag{3.3b}$$

$$\rho_2(-p) \equiv \sum_k a^*_{2\,k} a_{2\,k+p} \tag{3.4a}$$

$$= \sum_{k<-p} b^*_k b_{k+p} + \sum_{-p\le k<0} b^*_k c^*_{k+p} + \sum_{k>0} c_k c^*_{k+p}. \tag{3.4b}$$

Equations (3.1a)–(3.4a) give the density operators in the original representation, so let us calculate in this language a commutator such as (assume $p \geq p' \geq 0$ for definiteness)

$$[\rho_1(-p), \rho_1(p')] = \sum_{k,k'} [a^*_{1\,k} a_{1\,k+p}, a^*_{1\,k'+p'} a_{1\,k'}]$$

$$= \sum_{k=-\infty}^{+\infty} a^*_{1\,k} a_{1\,k+p-p'} - \sum_{k=-\infty}^{+\infty} a^*_{1\,k+p'} a_{1\,k+p} = 0. \tag{3.5}$$

The zero result could have been expected by writing the operators in first quantization:

$$\rho_1(-p) = \sum_n e^{-ipx_n} \quad \text{and} \quad \rho_2(p) = \sum_m e^{ipy_m}, \tag{3.6}$$

whence they evidently commute. Nevertheless, the zero result is achieved in (3.5) only through the almost "accidental" cancellation of two operators, each of which may diverge in the field-theory limit when $N = \infty$. We now show that in that limit the operators in fact no longer cancel, by evaluating the commutator using form (b) for the density operators. It is a matter of only some minor manipulation to obtain the important new result:

$$[\rho_1(-p), \rho_1(p')] = [\rho_2(p), \rho_2(-p')]$$

$$= \delta_{p,p'} \sum_{-p<k<0} 1 = \frac{pL}{2\pi} \delta_{p,p'}, \quad (p' > 0). \tag{3.7a}$$

In addition,

$$[\rho_1(p), \rho_2(p')] = 0. \tag{3.7b}$$

A quick check is provided by evaluating the vacuum expectation value

$$\langle 0|\, [\rho_1(-p), \rho_1(p)]\, |0\rangle$$

$$= \sum_{-p<k,k'<0} \langle 0|\, c_k b_{k+p} b^*_{k'+p} c^*_{k'}\, |0\rangle = pL/2\pi, \tag{3.8}$$

which is exactly what is expected on the basis of the previous equation. Evidently the form (b) of the operators $(2\pi/pL)^{+\frac{1}{2}}\rho_1(+p)$ and $(2\pi/pL)^{+\frac{1}{2}}\rho_2(-p)$ have properties of boson raising operators [call them $A^*(p)$ and $B^*(-p)$] and $(2\pi/pL)^{+\frac{1}{2}}\rho_1(-p)$ and $(2\pi/pL)^{+\frac{1}{2}}\rho_2(+p)$ have properties of boson lowering operators [$A(p)$ and $B(-p)$], i.e.,

$$[A, B] = [A^*, B] = 0,$$
$$[A(p), A^*(p')] = [B(-p), B^*(-p)] = \delta_{p,p'}. \tag{3.9}$$

The B field is the continuation of the A field to negative p; therefore together they form a *single* boson field defined for all p.

The relationship of the $\rho(p)$'s to Luttinger's $N(x)$'s, L(25), is obtained by using (2.4):

$$N_1(x) = \psi^*_1(x)\psi_1(x) = \frac{1}{L}\sum_p \rho_1(p) e^{-ipx},$$
$$N_2(x) = \psi^*_2(x)\psi_2(x) = \frac{1}{L}\sum_p \rho_2(p) e^{-ipx}. \tag{3.10}$$

IV. SOLUTIONS OF THE MODEL HAMILTONIAN

Before making use of the results of the previous section, we remark that $\rho_1(+p)$ and $\rho_2(-p)$ are exact raising operators of H_0, and $\rho_1(-p)$ and $\rho_2(p)$ are exact lowering operators of H_0 corresponding to excitation energies p. That is,

$$[H_0, \rho_1(\pm p)] = \pm p \rho_1(\pm p),$$
$$[H_0, \rho_2(\pm p)] = \mp p \rho_2(\pm p). \tag{4.1}$$

The identification of the ρ's with boson operators made in the previous section suggested to us the possibility of constructing a new operator T which obeys the same equations (4.1), as H_0. This is indeed possible, if we define T as follows:

$$T \equiv \frac{2\pi}{L}\sum_{p>0} \{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\} \tag{4.2}$$

[the ρ's being defined here and in the remainder of the paper by Eqs. (3.1b)—(3.4b), i.e., always in the hole-particle representation]. It follows that

$$[T, \rho_1(\pm p)] = \pm p \rho_1(\pm p) \tag{4.3}$$

as required, and similarly for $\rho_2(\mp p)$. Therefore, let us decompose H into two parts

$$H = H_1 + H_2 \tag{4.4}$$

with

$$H_1 = H_0 - T = \Big\{\sum_k |k|\,(b^*_k b_k + c^*_k c_k)$$
$$- \frac{2\pi}{L}\sum_{p>0} \{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\}\Big\}, \tag{4.5}$$

and

$$H_2 = H' + T$$
$$= \frac{1}{L}\Big[2\lambda \sum_{p>0} \{v(p)\rho_1(-p)\rho_2(p) + v(-p)\rho_1(p)\rho_2(-p)\}$$
$$+ 2\pi \sum_{p>0} \{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\}\Big] \tag{4.6}$$

with $v(p)$ = real, even function of p. By actual construction, all the ρ operators which appear in H_2

commute with H_1. This will be an important feature in constructing an exact solution of the model. We define an Hermitian operator S,

$$S = \frac{2\pi i}{L} \sum_{\text{all } p} \frac{\varphi(p)}{p} \rho_1(p)\rho_2(-p), \tag{4.7}$$

where $\varphi(p)$ is also a real, even, function of p to be determined subsequently by imposing a condition that the unitary transformation e^{iS} diagonalize H_2. First we evaluate the effect of such a transformation on various operators. It commutes with H_1,

$$e^{iS}H_1e^{-iS} = H_1 = H_0 - T, \tag{4.8}$$

because both ρ_1 and ρ_2 appearing in S commute with H_1, as noted above. In the following, p can have either sign:

$$e^{iS}\rho_1(p)e^{-iS} = \rho_1(p)\cosh\varphi(p) + \rho_2(p)\sinh\varphi(p), \tag{4.9}$$

$$e^{iS}\rho_2(p)e^{-iS} = \rho_2(p)\cosh\varphi(p) + \rho_1(p)\sinh\varphi(p). \tag{4.10}$$

We have verified that this transformation is a proper unitary transformation and preserves commutation relations (3.7) as well as anticommutation relations (2.5), and the reader may easily check this point. H_2 is brought into canonical form by requiring that in (exp iS) H_2 (exp $-iS$) there be no cross terms such as $\rho_1(p)\rho_2(-p)$. This leads to the equation

$$\tanh 2\varphi = -\lambda v(p)/\pi, \tag{4.11}$$

which cannot be obeyed unless

$$|\lambda v(p)| < \pi \quad \text{for all} \quad p. \tag{4.12}$$

Equation (4.12) serves to limit the magnitude of potentials capable of having well-behaved solutions (e.g., a real ground-state energy). For the more realistic potentials discussed in the Appendix, there is also a more realistic bound on $v(p)$: there, $v(p)$ may not be *too* attractive, but it can have any magnitude when it is repulsive, i.e., positive.

With the choice of φ in (4.11), the evaluation of H_2 becomes

$$e^{iS}H_2e^{-iS} = \frac{2\pi}{L} \sum_{p>0} \operatorname{sech} 2\varphi(p)\{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\} - \sum_{p>0} p(1 - \operatorname{sech} 2\varphi). \tag{4.13a}$$

The second term is the vacuum renormalization energy

$$W_1 = -\sum_{p>0} p(1 - \operatorname{sech} 2\varphi) = \frac{L}{2\pi}\int_0^\infty dp\, p\left\{\left(1 - \frac{\lambda^2 v^2(p)}{\pi^2}\right)^{\frac{1}{2}} - 1\right\}. \tag{4.13b}$$

It may be expanded in powers of λ to effect a comparison with Goldstone's many-body perturbation theory[4]; we have checked that they agree to third order.

The problem is now formally solved, for we can find all the eigenfunctions and eigenvalues by studying Eqs. (4.4), (4.8), and (4.13). First notice that the operator T does not depend upon the interaction and that if there is *no interaction* we could write the Hamiltonian either as

$$H = H_0, \tag{4.14a}$$

or as

$$H = (H_0 - T) + T = H_1 + H_2. \tag{4.14b}$$

Since H_1 and H_2 commute, every eigenstate, Ψ, of H may be assumed to be an eigenfunction of H_1 and H_2 separately. Moreover, Ψ may also be assumed to be an eigenfunction of each $\alpha_p = A_p^+A_p$ and $\beta_p = B_{-p}^+B_{-p}$ for all $p > 0$, since these operators commute with H and $\mathfrak{N}$.

Evidently (4.14a) and (4.14b) provide two different ways of viewing the noninteracting spectrum. H_0 is quite degenerate: the raising operators of H_0 are the b^+'s and c^+'s. By requiring that Ψ also be an eigenstate of α_p, β_p and H, we are merely attaching quantum numbers to the degenerate levels of H_0. If $\alpha_p\Psi = n_p\Psi$ and $\beta_p\Psi = m_p\Psi$ (where n_p and m_p are of course integers), we say that we have n_p plasmons of momentum p and m_p plasmons of momentum $-p$. With no interaction the energy of a plasmon is

$$\epsilon(p) = |p|. \tag{4.15}$$

We may speak of H_1 as the quasiparticle part of the Hamiltonian; in H_1 the operator T plays the role of subtracting the plasmon part of the energy from H_0.

When we turn on the interaction, the above description of the energy levels is still valid, except that now we are *forced* to use the form (4.14b) because H_2 is no longer T. The degeneracy of H is partially removed by the interaction, because now the energy of a plasmon is

$$\epsilon'(p) = |p| \operatorname{sech} 2\varphi(p). \tag{4.16}$$

Notice that the plasmon energy is always *lowered* [and therefore the plasmons cannot propagate faster than the speed of light $c = 1$, i.e., $d\epsilon'/dp \leq 1$. In the more realistic case discussed in the Appendix, the plasmon energy *can* be increased by the interaction although $d\epsilon'/dp \leq 1$ is always obeyed.] by the interaction; if (4.12) is violated the plasmon energy is no longer real and the system becomes unstable. Note, there are no plasmons in the ground state, so that W_1 (4.13), is the shift in the ground-state energy of the system.

There is one important point, however, that requires some elucidation. We would like to be able to say that in view of the fact that H_1, $\alpha(p)$, and $\beta(p)$

conserve particle number, the most general energy level of H (fixed N_0) is the sum of *any* energy of H_1 (same N_0, and no plasmons) plus *any* (plasmon) energy of H_2 (note: the plasmon spectrum is independent of N_0). Were we dealing with a finite-dimensional vector space, such a statement would not be true, for even though H_1 and H_2 commute they could not possibly be independent. Thus, if H_2 had n eigenvalues $e_1, \cdots, e_n$, and if H_1 had an equal number $E_1, \cdots, E_n$ the general total eigenvalue would not be *any* combination of $e_i + E_i$ for this would give too many values (viz. n^2 instead of n.) But we are dealing with an infinite-dimensional Hilbert space and the additivity hypothesis is in fact true for the present model.

To prove this assertion we consider any eigenstate Ψ which is necessarily parameterized by the integers n_p and m_p. Consider the state $\Phi = \{\prod_p (A_p)^{n_p}(B_p)^{m_p}\}\Psi$. The state Φ is nonvanishing and has quantum numbers $n_p = 0 = m_p$. It is also an eigenstate of H_1 with energy $E_1(\Psi)$. In addition (and this is the important point) the state Ψ may be recovered from Φ by the equation

$$\Psi = \text{const} \times \{\prod_p (A_p^+)^{n_p}(B_p^+)^{m_p}\}\Phi.$$

To every state Ψ, therefore, there corresponds a *unique* state Φ from which it may be obtained using raising operators. Conversely, to any eigenstate of H_1 (for fixed N_0) we may apply raising operators as often as we please and obtain a new (nonvanishing) eigenstate. Thus the general energy is an arbitrary sum of quasiparticle and plasmon energies.

It may be wondered where we used the fact that the Hilbert space is infinite-dimensional in the above proof. The answer lies in the boson commutation relations of the A's and B's. It is impossible to have such relations in a finite-dimensional vector space.

The eigenvalues corresponding to these states Φ will be labeled in some order, E_i $(i = 1, 2, \cdots)$, so that the total canonical partition function $Z(\lambda)$ and the free energy $F(\lambda)$ are given by

$$Z(\lambda) = e^{-F(\lambda)/kT} = (\sum_i e^{-E_i/kT})(e^{-W_1/kT}) \prod_{\substack{\text{all } p \\ \neq 0}} \left(\sum_{n=0}^{\infty} e^{-n\epsilon'(p)/kT}\right). \tag{4.17}$$

The first factor is difficult to evaluate directly. However it can be obtained circuitously by noting that the energies E_i are independent of λ and therefore

$$Z(0) = e^{-F(0)/kT} = (\sum_i e^{-E_i/kT}) \prod_{\substack{\text{all } p \\ \neq 0}} \left(\sum_{n=0}^{\infty} e^{-n\epsilon(p)/kT}\right). \tag{4.18}$$

But the second factor can be trivially evaluated, as can $F(0)$ = free energy of noninteracting fermions. Therefore we use (4.18) to eliminate the trace involving the E_i's in (4.17), with the final result:

$$F(\lambda) = F(0) + W_1 + 2kT \sum_{p>0} \ln \{(1 - e^{-\epsilon'(p)/kT})/(1 - e^{-\epsilon(p)/kT})\}, \tag{4.19}$$

where ϵ and ϵ' are given in (4.15) and (4.16). It is noteworthy that the ground state and free energy both diverge in the case of a δ-function potential.

V. EVALUATION OF THE MOMENTUM DISTRIBUTION

In this section we calculate the mean number of particles with momentum k. This quantity is $\bar{n}_k$ and is the expectation value of

$$n_k = b_k^+ b_k \tag{5.1}$$

in the ground state. Since $\bar{n}_k$ is an even function of k we need only consider $k > 0$, and it is further convenient to introduce a Fourier transform so that [using (2.4)]

$$\bar{n}_k = \frac{1}{L} \int_0^L\int ds\, dt\, e^{ik(s-t)} I(s, t). \tag{5.2}$$

Here

$$I(s, t) = \langle\Psi|\, \psi_1^+(s)\psi_1(t)\, |\Psi\rangle = \langle\Psi_0|\, e^{iS}\psi_1^+(s)e^{-iS}e^{iS}\psi_1(t)e^{-iS}\, |\Psi_0\rangle, \tag{5.3}$$

where S is given by (4.7), Ψ is the new ground state, and Ψ_0 is the noninteracting ground state which is filled with b particles between $-k_F$ and k_F and has no holes (or c particles). This assignment depends on there having been no level crossing, which can be readily verified using (4.7)–(4.13).

In order to calculate the quantity $e^{iS}\psi_1(t)e^{-iS}$ we introduce the auxiliary operator

$$f_\sigma(t) = e^{i\sigma S}\psi_1(t)e^{-i\sigma S}, \tag{5.4}$$

where σ is a c number. We observe that $f_1(t)$ is the desired quantity while

$$f_0(t) = \psi_1(t). \tag{5.5}$$

In addition,

$$\partial f/\partial\sigma = e^{i\sigma S} i[S, \psi_1(t)]e^{-i\sigma S} = e^{i\sigma S}[2\pi/L \sum_p \rho_2(-p)\varphi(p)p^{-1}e^{ipt}]e^{-i\sigma S} f_\sigma(t), \tag{5.6}$$

where we have used the commutation relations (3.7) as well as the fact that ψ_1 commutes with ρ_2. Equa-

tion (5.6) is a differential equation for $f_\sigma(t)$ and (5.5) is the boundary condition. The solution is

$$f_\sigma(t) = W_\sigma(t)R_\sigma(t)\psi_1(t), \tag{5.7}$$

where

$$W_\sigma(t) = \exp\{2\pi/L \sum_{p>0} [\rho_1(-p)e^{ipt} - \rho_1(p)e^{-ipt}]p^{-1}[\cosh \sigma\varphi(p) - 1]\} \tag{5.8}$$

and

$$R_\sigma(t) = \exp\{2\pi/L \sum_{p>0} [\rho_2(-p)e^{ipt} - \rho_2(p)e^{-ipt}]p^{-1} \sinh \sigma\varphi(p)\} \tag{5.9}$$

The reader may verify that (5.7) satisfies (5.5) and (5.6) by using the commutation relations (3.7). We recall the well-known rule that

$$\exp(A + B) = \exp(A) \exp(B) \exp(-1/2[A, B]) \tag{5.10}$$

when $[A, B]$ commutes with A and B. From here on we shall set $\sigma = 1$ and drop it as a subscript. We note that since $\rho_1(p)^+ = \rho_1(-p)$ and $\rho_2(p)^+ = \rho_2(-p)$,

$$R^+(t) = R^{-1}(t) \quad \text{and} \quad W^+(t) = W^{-1}(t). \tag{5.11}$$

We also note that R and W commute with each other. Thus, (5.3) becomes

$$I(s, t) = \langle\Psi_0| \psi_1^+(s)R^{-1}(s)W^{-1}(s)W(t)R(t)\psi_1(t) |\Psi_0\rangle = I_1(s, t)I_2(s, t), \tag{5.12}$$

where

$$I_1(s, t) = \langle\Psi_1| \psi_1^+(s)W^{-1}(s)W(t)\psi_1(t) |\Psi_1\rangle, \quad I_2(s, t) = \langle\Psi_2| R^{-1}(s)R(t) |\Psi_2\rangle. \tag{5.13}$$

We have used the fact that the ground state is a product state: $\Psi_0 = \Psi_1 * \Psi_2$ where Ψ_1 is a state of the "1" field and Ψ_2 is a state of the "2" field. Ψ_1 is filled with b particles up to $+k_F$ and has no c particles; Ψ_2 is filled with b particles down to $-k_F$ and has no c particles.

Now, using the definition (5.8) and the rule (5.10) we easily find that

$$W^{-1}(s)W(t) = W_-(s, t)W_+(s, t)Z_1(s, t), \tag{5.14}$$

with

$$W_+(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_1(-p)[\cosh \varphi(p) - 1] \times p^{-1}(e^{ipt} - e^{ips})\},$$

$$W_-(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_1(p)[\cosh \varphi(p) - 1] \times p^{-1}(e^{-ips} - e^{-ipt})\},$$

$$Z_1(s, t) = \exp\{2\pi/L \sum_{p>0} [\cosh \varphi(p) - 1]^2 \times p^{-1}(e^{ip(s-t)} - 1)\}. \tag{5.15}$$

Likewise,

$$R^{-1}(s)R(t) = R_-(s, t)R_+(s, t)Z_2(s, t), \tag{5.16}$$

with

$$R_+(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_2(p)[\sinh \varphi(p)] \times p^{-1}(e^{-ips} - e^{-ipt})\},$$

$$R_-(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_2(-p)[\sinh \varphi(p)] \times p^{-1}(e^{ipt} - e^{ips})\},$$

$$Z_2(s, t) = \exp\{2\pi/L \sum_{p>0} [\sinh \varphi(p)]^2 \times p^{-1}(e^{ip(t-s)} - 1)\}. \tag{5.17}$$

We see at once from the definition (3.1b), (3.2b), of $\rho_1(p)$ that, for $p > 0$, $\rho_1(-p) |\Psi_1\rangle = 0$. Similarly $\langle\Psi_1| \rho(p) = 0$, $\rho_2(p) |\Psi_2\rangle = 0$, and $\langle\Psi_2| \rho_2(-p) = 0$. Hence,

$$I_2(s, t) = Z_2(s, t)$$

and

$$I_1(s, t) = Z_1(s, t)\langle\Psi_1| W_-^{-1}\psi_1^+(s)W_-W_+\psi_1(t)W_+^{-1} |\Psi_1\rangle. \tag{5.18}$$

If we now define

$$h_+(y) = 2\pi/L \sum_{p>0} [\cosh \varphi(p) - 1] \times p^{-1}(e^{ipt} - e^{ips})e^{-ipy},$$

$$h_-(y) = 2\pi/L \sum_{p>0} [\cosh \varphi(p) - 1] \times p^{-1}(e^{-ipt} - e^{-ips})e^{ipy}, \tag{5.19}$$

combining (3.10) and (5.15) we have that

$$W_+(s, t) = \exp \int_0^L N_1(y)h_+(y)\, dy, \quad W_-(s, t) = \exp -\int_0^L N_1(y)h_-(y)\, dy. \tag{5.20}$$

Since

$$[\psi_1(x), N_1(y)] = \delta(x - y)\psi_1(x), \quad [\psi_1^+(x), N_1(y)] = -\delta(x - y)\psi_1^+(x), \tag{5.21}$$

it follows that

$$W_+(s, t)\psi_1(t)W_+^{-1}(s, t) = \psi_1(t) \exp[-h_+(t)], \quad W_-^{-1}(s, t)\psi_1^+(s)W_-(s, t) = \psi_1^+(s) \exp[+h_-(s)]. \tag{5.22}$$

Finally,

$$\langle\Psi_1|\ \psi_1^+(s)\psi_1(t)\ |\Psi_1\rangle = 1/L \sum_{p\le k_F} e^{ip(t-s)} \equiv Z_3(s,t). \tag{5.23}$$

Combining all these results, we conclude that

$$I(s,t) = Z_0(s,t)Z_1(s,t)Z_2(s,t)Z_3(s,t), \tag{5.24}$$

where

$$\begin{aligned} Z_0(s,t) &= \exp\,(h_-(s) - h_+(t)) \\ &= \exp\,\{-4\pi/L \sum_{p>0} [\cosh\varphi(p) - 1] \\ &\qquad \times (1 - e^{ip(s-t)})\}. \end{aligned} \tag{5.25}$$

In order to make a comparison with Luttinger's calculation of $\bar{n}_k$, we first observe that the functions $Z_i(s,t)$ are really functions of $r = s - t$ and that they are periodic in s and t in $(0, L)$. We then define the functions $G(r)$ and $Q(r)$ as follows:

$$\exp\,[-Q(r)] \equiv G(r) \equiv Z_0(r)Z_1(r)Z_2(r). \tag{5.26}$$

Substituting (5.26), (5.24), and (5.23) into (5.2) we obtain

$$\bar{n}_k = 2\pi/L \sum_{p\le k_F} F(k-p), \tag{5.27}$$

where

$$F(k) = 1/2\pi \int_{-\frac{1}{2}L}^{\frac{1}{2}L} dr\, e^{ikr} e^{-Q(r)} \tag{5.28}$$

$$\cong 1/2\pi \int_{-\infty}^{\infty} dr\, e^{ikr} e^{-Q(r)}. \tag{5.29}$$

In (5.29) we have passed to the bulk limit N, $L \to \infty$, not an approximation.

At this point our expression for $\bar{n}_k$ is formally the same as Luttinger's [cf. L (52), L (69)]. The difference is that our Q is different from his. He obtains Q by evaluating an infinite Toeplitz determinant with the result that [L (70)]

$$Q(r) = \lambda^2/2\pi^2 \int_0^\infty dp\, \frac{1-\cos pr}{p}\, |v(p)|^2. \quad \text{(Luttinger)} \tag{5.30}$$

Our Q, which is the correct one to use, is obtained by combining (5.15), (5.17), and (5.25), replacing sums by integrals in the usual way, and using the definition (4.11) of $\varphi(p)$. The result is

$$Q(r) = \lambda^2/2\pi^2 \int_0^\infty dp\, \frac{1-\cos pr}{p}\, |u(p)|^2, \tag{5.31}$$

where

$$|u(p)|^2 = (2\pi^2/\lambda^2)\{(1 - (\lambda v(p)/\pi)^2)^{-\frac{1}{2}} - 1\}. \tag{5.32}$$

It is worth noting that (5.30) agrees with (5.31) to leading order in λ^2.

Since we have not yet specified $v(p)$, we may now follow Luttinger's discussion from this point on with the proviso that we use the correct (λ dependent) $u(p)$ instead of $v(p)$. The reader is referred to pages 1159 and 1160 of Luttinger's paper.

There are two main conclusions one can draw. The first is that if we start with a δ-function interaction [so that $v(p)$ and hence $u(p)$] are constants, it can be shown that $\bar{n}_k = \frac{1}{2}$ for all k. Such a result is quite unphysical, but it is not unreasonable because the ground-state energy W (4.13a) diverges when $v(p) =$ constant at large p. Also, the result would be the same if we started with the more physical interaction

$$H' = 1/L \sum_p \{\rho_1(p) + \rho_2(p)\}\{\rho_1(-p) + \rho_2(-p)\}v(p)$$

discussed in the Appendix. This is indeed unfortunate, because relativistic field theories usually begin with local (δ-function) interactions.

The second conclusion is that if one makes a reasonable assumption about $v(p)$, and hence about $u(p)$ and $Q(r)$, one finds that for k in the vicinity of k_F, $\bar{n}_k$ behaves like

$$\bar{n}_k \sim d - e\ |k - k_F|^{2\alpha}\ \sigma(k - k_F), \tag{5.33}$$

where

$$\begin{aligned} \sigma(k) &= 1, \qquad k > 0 \\ &= -1, \qquad k < 0 \end{aligned} \tag{5.34}$$

and d, e, and α are certain positive constants. Now in Luttinger's calculation

$$\alpha = \lambda^2/4\pi^2 v(0)^2, \quad \text{(Luttinger)} \tag{5.35}$$

[cf. L(75)], where $v(0) \equiv \lim_{p\to 0} v(p)$.

If $2\alpha < 1$, then the conclusion to be drawn is that although the interaction removes the discontinuity in $\bar{n}_k$ at the Fermi surface, we are left with a function that has an infinite slope there. There is, so to speak, a residual Fermi surface. In Sec. IV of his paper, Luttinger shows that at least for one example of $v(p)$ perturbation theory gives the same qualitative result as (5.33) with the same value of α, (5.35).

If, on the other hand, $2\alpha > 1$ then there is no infinite derivative at the Fermi surface. $\bar{n}_k$ is perfectly smooth there (although, technically speaking, it is nonanalytic unless $2\alpha =$ odd integer.) In this case virtually all trace of the Fermi surface has been eliminated. But notice that the correct α to use is obtained by replacing $v(0)$ by $u(0) \equiv \lim_{p\to 0} u(p)$ in (5.35), i.e.,

$$2\alpha = \{1 - [\lambda v(0)/\pi]^2\}^{-\frac{1}{2}} - 1. \quad (5.36)$$

Thus, even subject to the requirement that $|\lambda v(0)|$ be less than π, 2α can become as large as one pleases. Yet perturbation theory predicts (5.35) which yields 2α always less than $\frac{1}{2}$.

We may conclude that a strong enough interaction can eliminate the Fermi surface, while perturbation theory predicts that is always there.

VI. DIELECTRIC CONSTANT

Because the response to external fields of wave vector q only depends on an interaction expression linear in the density operators, we can immediately obtain for the generalized static susceptibility function or *dielectric constant* (response ÷ driving force), for any temperature, T

$$\chi_\lambda(q, T) = \chi_0(q, T)\{\sinh \varphi(q) + \cosh \varphi(q)\}^2 \cosh 2\varphi_q = \chi_0(q, T)\frac{1}{1 + \lambda v(q)/\pi} \quad (6.1)$$

in terms of the "unperturbed" susceptibility $\chi_0(q, T)$. It is also a simple exercise to calculate exactly the time dependent susceptibility in terms of the "unperturbed" quantity.

It is interesting to note that the susceptibility can diverge (which is symptomatic of a phase transformation) only for

$$\lambda v(q) \to -\pi, \quad (6.2)$$

i.e. only for sufficiently *attractive* interactions and not for repulsive [$v(q) > 0$] interactions.

Recently Ferrell[6] advanced plausible arguments why a one-dimensional metal cannot become superconducting. We can prove this rigorously in the present model. The electron–phonon interaction is

$$H_{\text{el-ph}} = \sum_p g(p)[\rho_1(p) + \rho_2(p)]\cdot[\xi_p + \xi^+_{-p}], \quad (6.3)$$

where ξ and ξ^+ are the phonon field operators. In the "filled-sea" limit this coupling is bilinear in harmonic-oscillator operators, and therefore the Hamiltonian continues to be exactly diagonalizable. The new normal modes can be calculated and there is found to be no phase transition at any finite temperature.

APPENDIX

We shall be interested in extending Luttinger's model in two ways. Firstly, we note that the restriction $\bar{V} = 0$ is really not necessary. Turning back to Eqs. (2.13) *et seq.* we impose periodic boundary conditions $\Psi(\cdots, x_i + L, \cdots) = \Psi(\cdots, x_i, \cdots)$, and find that

$$(q + N\lambda\bar{V}) \text{ and } (k + M\lambda\bar{V}) = 2\pi/L \times \text{integer} \quad (A1)$$

replace the usual condition (2.16), where N = number of "1" particles and M = number of "2" particles. However, when $N, M \to \infty$ in the field-theoretic limit the problem evidently becomes ill-defined unless $\bar{V} \equiv 0$.

A less trivial observation concerns the form of the interaction potential. There is no reason to restrict it to the form $\propto \rho_1\rho_2$, and in fact the more realistic two-body interaction

$$H' = \frac{\lambda}{L}\sum_p v(p)\{\rho_1(-p) + \rho_2(-p)\}\{\rho_1(p) + \rho_2(p)\} \quad (A2)$$

is fully as soluble as the one assumed in the text, for any strength positive $v(p)$, and provided only

$$\lambda v(p) > -\tfrac{1}{2}\pi, \quad (A3)$$

i.e. provided no Fourier component is *too* attractive. The shift in the ground-state energy is now given by

$$W_2 = \sum_{p>0} p\left\{\left(1 + \frac{2\lambda v(p)}{\pi}\right)^{\frac{1}{2}} - 1\right\}. \quad (A4)$$

The plasmon energy is now

$$\epsilon''(p) \equiv |p|\,(1 + 2\lambda v(p)/\pi)^{\frac{1}{2}} \quad (A5)$$

and *for the important case of the Coulomb repulsion,* $v(p) = p^{-2}$, the plasmons describe a relativistic boson field with mass

$$m^* \equiv (2\lambda/\pi)^{\frac{1}{2}} \quad (A6)$$

and dispersion

$$\epsilon''(p) = (p^2 + m^{*2})^{\frac{1}{2}}. \quad (A7)$$

Here, too, $d\epsilon''/dp < 1$.

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[6] R. A. Ferrell, Phys. Rev. Letters **13**, 330 (1964).

[7] P. Jordan, Z. Physik **93**, 464 (1935); **98**, 759 (1936); **99**, 109 (1936); **102**, 243 (1936); **105**, 114 (1937); **105**, 229 (1937). M. Born and N. Nagendra-Nath, Proc. Ind. Acad. Sci. **3**, 318 (1936). A. Sokolow, Phys. Z. der Sowj. **12**, 148 (1937).

Adiabatic Particle Orbits in Discontinuous Fields

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The invariance properties of the action integral $J = \oint p\,dq$ are studied for the motion of charged particles in one-dimensional electromagnetic fields. Attention is concentrated on those situations where the field gradients become large. Whereas in the case of smooth fields and finite gradients the asymptotic theory of the one-dimensional oscillator as developed by Gardner and by Lenard applies, the presence of large gradients, requires a special treatment. The present considerations are restricted to cases where the strong field variation is confined to a small region such that the transition can be approximated by a discontinuity. It is shown that for time intervals of order $1/\epsilon$, J is an adiabatic invariant of at least order $\epsilon^{\frac{1}{2}}$, ϵ measuring the time variation of the fields. As an example, the motion of high-speed particles through a plane discontinuity is shown to be adiabatic in that sense. Consequently, the initial and the final magnetic moments differ only slightly.

1. INTRODUCTION

THE invariance properties of the action integral $J = \oint p\,dq$ play an important role in plasma theory. J has been studied by many authors for various Hamiltonian systems. It is commonly assumed, however, that (at least for almost all times) the Hamiltonian must be smooth, which in most cases is understood in the sense of infinite differentiability. In the work of Gardner[1] and in other studies explicitly concerned with particle orbits in three-dimensional electromagnetic fields[2-4] it is assumed, in addition, that the field gradients must be small.

Here we consider a special class of situations, where the latter condition can be dropped. Our main assumption is that the fields must be one dimensional. A typical example of this situation occurs when particles drift through a plane shock front (as discussed in Sec. 4) or when a collision-free cylindrical plasma is confined by an axial magnetic field (θ-pinch geometry). Particularly, we are concerned with situations where large field variations are involved.

In the case of smooth fields with finite gradients, the asymptotic theory of the one-dimensional oscillator applies, as developed by Lenard[5] and in the first part of Gardner's work[1] where a different method is used.[6] From their results we immediately obtain the following property: If the Hamiltonian H is such that for any fixed time t the curves $H =$ const. form a set of closed curves in the p–q plane with the topology of concentric circles, and if H is sufficiently smooth and independent of time for $t \leq t_1$ and $t \geq t_2$, then the action integral (the integration is performed along a curve of constant H)

$$J = \oint p\,dq \tag{1.1}$$

is an adiabatic invariant in the sense that for any initial condition the difference ΔJ of the initial and the final value of (1.1) can be estimated by

$$|\Delta J| < M_n \epsilon^n, \qquad n = 1, 2, \cdots, \epsilon > 0, \tag{1.2}$$

where M_n is a positive constant depending on the exponent n but independent of ϵ (the scale of the time variation of H).

The required topological condition is in many cases satisfied if the magnetic field is unidirectional. J is computable in terms of H and the fields, which makes the invariance useful for practical applications.[7] The importance of this generalized invariance for one-dimensional and for almost one-dimensional fields was first pointed out by Grad.[8]

The invariance (1.2) holds for bounded field gradients and, particularly, in the limit of vanishing gradients and electric fields, where J is proportional to the magnetic moment W/B (W = kinetic energy, B = magnetic induction). In the case of unbounded field gradients and discontinuous fields, however, the previous studies of the one-dimensional oscillator fail to yield adiabatic invariance. Thus the question arises, whether or not an expression similar to (1.2)

[1] C. S. Gardner, Phys. Rev. **115**, 791 (1959).
[2] J. Berkowitz and C. S. Gardner, Comm. Pure Appl. Math. **12**, 501 (1959).
[3] G. Hellwig, Z. Naturforsch. **10a**, 508 (1955).
[4] M. Kruskal, Proc. Intern. Conf. Ionization Phenomena Gases, 3rd, Venice, 1957, p. 562.
[5] A. Lenard, Ann. Phys. (N. Y.) **6**, 261 (1959).
[6] See also Y. Watanabe, Progr. Theoret. Phys. (Kyoto) **27**, 653 (1962).
[7] M. Kruskal, J. Math. Phys. **3**, 806 (1962).
[8] H. Grad, "General Adiabatic Theory," TID-7520 (Pt. 2), 402 (1956).

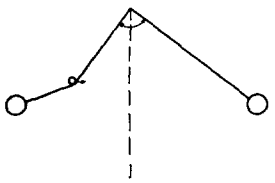

FIG. 1. A pendulum in a discontinuous force field.

can be obtained such that, for a given ϵ, ΔJ remains small when the field gradients become large.

It is the purpose of the present work to discuss the behavior of J under these circumstances. We restrict our considerations to the case in which the electromagnetic field has a discontinuity and is sufficiently smooth otherwise. This is believed to be a valid approximation for the case in which the field changes rapidly in a region small compared with a typical radius of curvature of the particle orbit.

Under the assumptions specified in the following section, the present problem reduces to analyzing a one-dimensional oscillator moving in a potential which is continuous but which may have discontinuous derivatives. A mechanical example is a pendulum, the thread of which is bent by a slowly moving pin (Fig. 1). Starting out in a way quite similar to that followed by Lenard[5] we show that J is an adiabatic invariant of at least order $\epsilon^{\frac{1}{2}}$.

2. ASSUMPTIONS AND DEFINITIONS

Denoting the physical time by t' we consider Hamiltonians of the form

$$H(p, q, t') = \tfrac{1}{2}p^2 + \psi(q, \epsilon t'), \tag{2.1}$$

with $\epsilon > 0$. This Hamiltonian clearly contains the plane and cylindrical cases mentioned above. We introduce

$$t = \epsilon t' \tag{2.2}$$

as a new time coordinate and postulate the following properties for $\psi(q, t)$:

(1) $\psi(q, t)$ is a continuous function of q and t.

(2) $\psi_q(q, t)$, $\psi_t(q, t)$ are continuous for $q \neq R(t)$ with a jump discontinuity at $q = R(t)$ where R, $\dot{R}$ are continuous and $\dot{R}$, $\ddot{R}$ bounded.

(3) There is a continuous function $q_0(t)$ such that for all t

$$\begin{aligned} \psi(q, t) = \psi_q(q, t) = 0 \quad &\text{for} \quad q = q_0(t), \\ \psi_q(q, t) \gtrless 0 \quad &\text{for} \quad q \gtrless q_0(t). \end{aligned} \tag{2.3}$$

Under these conditions the set of curves $H = \text{const.}$, which we call Γ_H, form a set of closed curves with the topology of concentric circles, H being zero at the center $(0, q_0)$ and increasing in any outward direction. The two points at which Γ_H intersects the q axis will be denoted by $\xi_1(H, t) \leq \xi_2(H, t)$ satisfying the equations

$$\psi(\xi_i, t) = H, \qquad i = 1, 2. \tag{2.4}$$

The action integral (1.1) then takes the form

$$J(p, q, t) = f(H, t) = 2^{\frac{1}{2}} \int_{\xi_1}^{\xi_2} [H - \psi(\xi, t)]^{\frac{1}{2}}\, d\xi. \tag{2.5}$$

It should be noted that the path of integration in (2.5) is a closed level curve of the "frozen Hamiltonian" and not the actual orbit, which in general is not closed.

As the H dependence of $f(H, t)$ is monotonic there is a uniquely defined inverse function

$$H = \phi(J, t). \tag{2.6}$$

Given two constants $H' < H''$ we postulate:

(4) There exist four numbers J', J'', H_0, H_1 such that

$$\begin{aligned} 0 < J' &\leq \min_t f(H', t) \\ J'' &\geq \max_t f(H'', t), \\ 0 < H_0 &\leq \min_t \phi\left(\frac{J'}{2}, t\right) \\ H_1 &\geq \max_t \phi(2J'', t), \end{aligned} \tag{2.7}$$

where, for simplicity, we choose the time interval considered to be infinite: $-\infty < t < +\infty$.

Now, we define the following domains in the p–q plane:

$$\begin{aligned} Q(t)&: \quad H_0 \leq H \leq H_1, \\ Q'(t)&: \quad \tfrac{1}{2}H_0 \leq H \leq 2H_1, \\ Q''(t)&: \quad 0 \leq H \leq 2H_1, \end{aligned} \tag{2.8}$$

and require:

(5) For $(0, q)$ in $Q'(t)$, $\psi_q(q, t)$ is bounded from below; for $(0, q)$ in $Q''(t)$, all first and second derivatives of ψ are bounded.

An "orbit" is characterized by any solution $p(t)$, $q(t)$ of the Hamiltonian equations of motion

$$\epsilon\, dq/dt = p, \qquad \epsilon\, dp/dt = -\psi_q; \tag{2.9}$$

$p(t)$ and $q(t)$ are continuous at $q(t) = R(t)$. When we write $J(t)$, $f(t)$, etc., instead of $J(p, q, t)$, $f(p, q, t)$, etc., p and q have been introduced as the coordinates of an orbit.

It should be mentioned that Condition 4 is not very restrictive. It is easily shown that 4 is satisfied if $\psi(q, t)$ for all t lies between two comparison functions proportional to $[q - q_0(t)]^2$.

3. PROOF OF THE INVARIANCE

We show that J is an adiabatic invariant in the following sense: Suppose the conditions specified in the preceding section are satisfied and at time t_1 the inequality

$$H' \leq H(t_1) \leq H'' \tag{3.1}$$

holds, then for any time $t_2 > t_1$ and ϵ sufficiently small

$$|J(t_2) - J(t_1)| < M_1\epsilon^{\frac{1}{2}}(t_2 - t_1) + M_2\epsilon \tag{3.2}$$

is satisfied.

We show this first under the additional assumption that for t in $[t_1, t_2]$

$$H_0 \leq H(t) \leq H_1 \tag{3.3}$$

holds, that is, that the orbit stays in $Q(t)$, see (2.8). Then, as a second step we show that (3.3) in fact is satisfied. Note, that for the present purpose it is not necessary to postulate time independence of the Hamiltonian for $t < t_1$ and $t > t_2$. (The same is true in the smooth case for the first order, but not for higher orders.)

Following Lenard,[5] we consider the Liouville equation written in the form

$$\epsilon\, \partial f/\partial t + |\nabla H|\, \partial f/\partial s = 0. \tag{3.4}$$

Here, the action integral J and the arc length s on the Γ curves have been introduced as new coordinates, replacing p and q. However, $\partial f/\partial t$ is still to be evaluated at a fixed point (p, q).

We first try to obtain an asymptotic expression of order ϵ for the function f. The formal expansion

$$f = f_0 + \epsilon f_1 + \cdots \tag{3.5}$$

introduced into (3.4) yields in the ϵ orders 0 and 1:

$$\partial f_0/\partial s = 0 \tag{3.6}$$

$$\partial f_1/\partial s = -(1/|\nabla H|)\, \partial f_0/\partial t. \tag{3.7}$$

A solution is given by

$$f_0 = J \tag{3.8}$$

$$f_1 = -\frac{1}{\sqrt{2}} \int_{\xi_1}^{q} \frac{\partial J}{\partial t} \frac{d\xi}{[H - \psi(\xi, t)]^{\frac{1}{2}}} + B(J, t), \tag{3.9}$$

where $B(J, t)$ is an arbitrary function of J and t.

In (3.9) and in the following expressions for f_1 we take $p > 0$; it is easily shown that $f_1(p, q, t) = -f_1(-p, q, t)$.

As we shall see, the presence of the discontinuity makes $\partial f_1/\partial t$ become infinite on the curve $H = \psi(R, t)$ so that the conditions

$$\oint_\Gamma \frac{\partial f_1}{\partial t} \frac{ds}{|\nabla H|} = 0, \tag{3.10}$$

$$\left|\frac{\partial f_1}{\partial t}\right| \text{ bounded}, \tag{3.11}$$

which have been used by Lenard [(3.10) is a condition on $B(J, t)$] cannot be imposed in our case, and we have to proceed in a different way. First, we drop (3.10) because this condition is only necessary to insure the single-valuedness of f_2, in which we are not interested. Instead we choose $B(J, t) \equiv 0$. From the differential equation (3.4) we can write

$$f = f_0 + \epsilon\left(f_1 - \int_{t_1}^{t} \frac{\partial f_1}{\partial t}\, dt\right), \tag{3.12}$$

where the integral is understood to be performed along the orbit passing through the point (p, q) at time t.

At least formally, (3.12) is an exact solution of (3.4) as may be verified by taking the time derivative of (3.12) along the orbit, observing that

$$\epsilon\left(f_1 - \int_{t_1}^{t} \frac{\partial f_1}{\partial t}\, dt\right) = \int_{t_1}^{t} |\nabla H| \frac{\partial f_1}{\partial s}\, dt + \epsilon f_1(t_1). \tag{3.13}$$

Now, suppose f_1 and the integral in (3.12) evaluated at $t = t_2$ are bounded:

$$|f_1| < M', \tag{3.14}$$

$$\left|\int_{t_1}^{t_2} \frac{\partial f_1}{\partial t}\, dt\right| < M'', \tag{3.15}$$

where M'' may depend on ϵ as the orbit does whereas M' is independent of ϵ. Then we obtain from (3.12)

$$|f(p, q, t_2) - f_0(p, q, t_2)| < (M' + M'')\epsilon. \tag{3.16}$$

This leads to an estimate on J in the following way: (3.4) requires that f remain constant on any orbit. So, using (3.8) and (3.12) we can write

$$\begin{aligned} f(t_2) = f(t_1) &= J(t_1) + \epsilon f_1(t_1), \\ f_0(t_2) &= J(t_2). \end{aligned} \tag{3.17}$$

From (3.16) with p and q taken on the orbit we obtain

$$|J(t_1) + \epsilon f_1(t_1) - J(t_2)| < \epsilon(M' + M'')$$

and with (4.13)

$$|J(t_2) - J(t_1)| < \epsilon(2M' + M''). \tag{3.18}$$

So it remains to show that (3.14) and (3.15) are

satisfied with a suitable ϵ dependence of M''. Using (2.5) and (3.9) we write f_1 in the form

$$f_1 = z_1(\xi_2, H, t)z_2(q, H, t) - z_1(q, H, t)z_2(\xi_2, H, t), \tag{3.19}$$

where

$$z_i(x, H, t) = \int_{\xi_1(H,t)}^{x} \frac{G_i(\xi, t)\, d\xi}{[H - \psi(\xi, t)]^{\frac{1}{2}}}, \quad i = 1, 2, \tag{3.20}$$

with

$$G_1(\xi, t) = \psi_t(\xi, t), \qquad G_2(\xi, t) \equiv 1. \tag{3.21}$$

In order to estimate z_i and $\partial z_i/\partial t$ it is convenient to integrate (3.20) by parts. The resulting expression, however, becomes meaningless at $x = q_0$, where ψ_q vanishes [see (2.3)]. So we break up the interval $[\xi_1, \xi_2]$ at the points

$$a_1(t) = \xi_1(\tfrac{1}{2}H_0, t), \qquad a_2(t) = \xi_2(\tfrac{1}{2}H_0, t) \tag{3.22}$$

and use the original representation (3.20) in the interval (a_1, a_2). Defining the functions

$$\phi_{i1}(x) = -2[H - \psi(x, t)]^{\frac{1}{2}}G_i(x, t)/\psi_q(x, t)$$

$$\phi_{i2}(x, y) = 2\int_x^y [H - \psi(\xi, t)]^{\frac{1}{2}}\left(\frac{G_i(\xi, t)}{\psi_q(\xi, t)}\right)_\xi d\xi \tag{3.23}$$

$$\phi_{i3}(x, y) = \int_x^y \frac{G_i(\xi, t)}{[H - \psi(\xi, t)]^{\frac{1}{2}}}\, d\xi,$$

we obtain

$\xi_1 \le x \le a_1$:

$$z_i = \phi_{i1}(x) + \phi_{i2}(\xi_1, x) + 2Y\Delta(G_i/\psi_q)\gamma,$$

$a_1 < x < a_2$:

$$z_i = \phi_{i1}(a_1) + \phi_{i2}(\xi_1, a_1) + \phi_{i3}(a_1, x) + 2Y\Delta(G_i/\psi_q)\gamma, \tag{3.24}$$

$a_2 \le x \le \xi_2$:

$$z_i = \phi_{i1}(a_1) + \phi_{i2}(\xi_1, a_1) + \phi_{i2}(a_1, a_2) + \phi_{i1}(x) - \phi_{i1}(a_2) + \phi_{i2}(a_2, x) + 2Y\Delta(G_i/\psi_q)\gamma,$$

where

$$Y = [H - \psi(R, t)]^{\frac{1}{2}}, \quad H \ge \psi(R, t), \qquad Y = 0, \quad H < \psi(R, t). \tag{3.25}$$

$\Delta(G_i/\psi_q)$ denotes the jump of G_i/ψ_q across the discontinuity and $\gamma = \gamma_1\gamma_2$ where

$$\gamma_1 = 1 \text{ for } \xi_1 < R \le x \text{ and } \gamma_1 = 0 \text{ otherwise}, \qquad \gamma_2 = 0 \text{ for } a_1 < R \le a_2 \text{ and } \gamma_2 = 1 \text{ otherwise}. \tag{3.26}$$

Observing from (3.19) that x equals q or ξ_2, we conclude from (3.24) that under the assumptions formulated in Sec. 2 all terms of z_i and $\partial z_i/\partial t$ are bounded except for those terms containing $\partial Y/\partial t$ which diverge for $H = \psi(R, t)$. {Note that $[H - \psi(q, t)]^{\frac{1}{2}} = p/2^{\frac{1}{2}}$, $[H - \psi(\xi_2, t)]^{\frac{1}{2}} = 0$, and $[H - \psi(x, t)]^{\frac{1}{2}} \ge (H_0/2)^{\frac{1}{2}}$ for $a_1 \le x \le a_2$.} Thus we write

$$|z_i| < U, \qquad |\partial z_i/\partial t| < W_1 + W_2\,|\partial Y/\partial t|, \qquad i = 1, 2 \tag{3.27}$$

where U, W_1, W_2 are positive constants, independent of ϵ.

Although $\partial Y/\partial t$ is not bounded, one can obtain an upper bound on $\int_{t_1}^{t_2} |\partial Y/\partial t|\, dt$:

$$\int_{t_1}^{t_2} \left|\frac{\partial Y}{\partial t}\right| dt < \frac{S_1}{\epsilon^{\frac{1}{2}}}(t_2 - t_1) + S_2\epsilon^{\frac{1}{2}}, \tag{3.28}$$

where S_1, S_2 are constants, independent of ϵ, t_1, t_2. The proof of (3.28) is given in the Appendix. Using (3.28) we conclude from (3.19) and (3.27) that (3.14) and (3.15) hold with

$$M' = 2U^2$$

$$M'' = 4UW_1(t_2 - t_1) + 4UW_2[S_1\epsilon^{-\frac{1}{2}}(t_2 - t_1) + S_2\epsilon^{\frac{1}{2}}].$$

Thus, from (3.18) we finally obtain (3.2) with $M_1 = 8US_1W_2$, $M_2 = 8U^2$ where for convenience, ϵ is restricted to

$$\epsilon < \min\,|(U/S_2W_2)^2, (S_1W_2/W_1)^2|.$$

It remains to show that (3.3) is satisfied. We assume that the orbit leaves the domain $Q(t)$ as defined in (2.8) during $[t_1, t_2]$. As we shall see, this leads to a contradiction. We first consider the case in which the boundary of $Q(t)$ crossed first, is the boundary $H = H_0$ and is crossed, say, at time $t = T_1 \le t_2$. We have with the aid of (2.7):

$$H(T_1) = H_0, \qquad J(T_1) \le \tfrac{1}{2}J' \tag{3.29}$$

while initially

$$J(t_1) \ge J', \tag{3.30}$$

as follows from (2.7) and (3.1). Since during the interval $[t_1, T_1]$ the orbit is still in $Q(t)$, (3.2) holds as shown before:

$$|J(T_1) - J(t_1)| < M_1\epsilon^{\frac{1}{2}}(T_1 - t_1) + M_2\epsilon \le M_1\epsilon^{\frac{1}{2}}(t_2 - t_1) + M_2\epsilon. \tag{3.31}$$

On the other hand, (3.29) and (3.30) lead to

$$|J(T_1) - J(t_1)| \ge J'/2$$

which contradicts (3.31) if ϵ is sufficiently small. So, the orbit cannot leave the domain $Q(t)$ by passing the boundary $H = H_0$. If the boundary $H = H_1$ is assumed to be crossed first, the argument runs similarly. This, then, completes the proof of (3.2) except for the estimate of (3.28) which is given in the Appendix.

Since the right-hand side of (3.2) goes to zero with $\epsilon \to 0$ for all orbits, J is an adiabatic invariant. According to the conventional terminology we have shown invariance of order $\frac{1}{2}$ because the leading term contains ϵ in that power.

We add a brief remark concerning higher-order invariance. While for general field situations only invariance of order $\frac{1}{2}$ seems to be possible by this method, there are examples in which invariance of order 1 can be obtained, in spite of the presence of discontinuities. This, for example, is true for the plane discontinuity moving with constant speed as discussed in Sec. 4. However, as we do not need this improvement there, we shall ignore it and, for sake of brevity, use the general result (3.2).

In the present approach the higher-order invariance is excluded by the presence of the term Y, the time derivative of which becomes large if H approaches $\psi(R, t)$. However, if R remains sufficiently close to the center q_0 of the Γ curves, $\partial Y/\partial t$ remains finite and higher-order invariance can be obtained. On the other hand, for a particle which did not hit the front before and starts passing it, the equation $H = \psi(R, t)$ is satisfied at least once and we cannot obtain higher-order results.

In cases where the nth derivatives of H have jump discontinuities (all lower derivatives being continuous), the present procedure may be used to obtain invariance of order $n - \frac{1}{2}$ instead of order $n - 1$. There, however, the gain of one half order will be less interesting than in the case $n = 1$ treated here, where without that extra half order, there would be no invariance at all.

In some cases where the magnetic field goes through zero, (2.3) does not hold and some orbits may become nonadiabatic. The case of a homogeneous magnetic field which goes through zero has been studied by Tamor.[9]

4. PARTICLES PASSING THROUGH A PLANE SHOCK FRONT

As an example, we consider particles moving through a plane discontinuity separating two regions of constant homogeneous magnetic field. On either side of the front the field vector **B** points into the same direction parallel to the front. The front moves along its normal direction with constant speed, inducing an electric field **E** perpendicular to **B** and parallel to the front.

In speaking of a shock front, we must keep in mind that a discontinuity probably is not a realistic model for any actual collision-free shock wave, because it ignores the oscillatory structure behind the front as established by C. S. Morawetz.[10]

Particle orbits of the kind considered here have been discussed previously by E. N. Parker[11] in connection with acceleration mechanisms for particles in electromagnetic fields. Although adiabatic invariance is assumed, it so far seems established only by numerical calculations.

We treat the present problem in two steps. First, we show that the particle can stay with the front only for a finite time and is left behind afterwards. In the second step this result is used to establish that the change of the magnetic moment caused by the passing front is small for small front velocities.

Before giving a more precise formulation of these properties we observe that a particle separated from the front by a sufficiently large distance performs the familiar drift motion in crossed fields, or, if the electric field vanishes, moves around in circles. Particles in this state of motion will be called "separated"; particles which are not separated are "connected" (to the front).

Looking at the particle motion in a frame of reference in which E vanishes on one side of the discontinuity, we can state the point to be shown in the following way ($t' = t/\epsilon$ as before is the physical time):

(i) Suppose a particle passes through the front at time t'_{I}. Then, for sufficiently small front velocities $|c|$, a positive constant N can be found such that the particle cannot pass through the front again at any time $t'_{\mathrm{II}} = t'_{\mathrm{I}} + \theta$ with

$$\theta > N/|c|. \tag{4.1}$$

(ii) Suppose a particle initially separated from the front passes through the front at $t' = \tau_{\mathrm{I}}$ for the first time, and $|c|$ is sufficiently small. Then, at any time $t' > \tau_{\mathrm{I}} + N/|c|$ the particle is separated again, now drifting (or circling) on the other side of the front and will stay so for any later time. The difference between the initial and the final magnetic moment H/B is of order $|c|^{\frac{1}{2}}$ or of higher order.

[9] S. Tamor, J. Nucl. Energy **C1**, 199 (1960).

[10] C. S. Morawetz, Phys. Fluids **4**, 988 (1961).

[11] E. N. Parker, Phys. Rev. **109**, 1328 (1958).

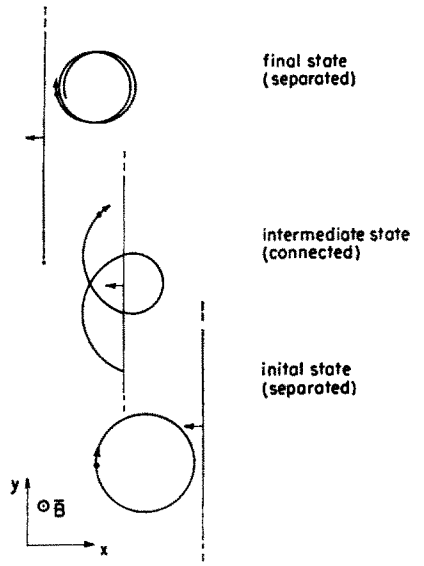

FIG. 2. Particles passing through a plane discontinuity. (The magnetic field jumps by a factor of 2.)

We choose a Cartesian coordinate frame as indicated in Fig. 2 and take $E = 0$ in $x < R$. Then the Hamiltonian can be written as (mass and charge are eliminated by choosing suitable dimensionless variables):

$$H = \tfrac{1}{2}p_x^2 + \psi(x, t),$$
$$\psi(x, t) = \begin{cases} \tfrac{1}{2}B_1^2(x - x_0)^2 & \text{for } x < R(t), \\ \tfrac{1}{2}[B_2 x - R(B_2 - B_1) - B_1 x_0]^2 & \text{for } x > R(t). \end{cases} \tag{4.2}$$

x_0 denotes a constant of motion which, geometrically, is the position of the center of the circular orbit section in $x < R$. $B_1 > 0$, $B_2 > 0$ are the magnetic field strengths in $x < R$ and $x > R$ respectively. The speed of the front is given by

$$c = \epsilon\dot{R}. \tag{4.3}$$

Since only the product of ϵ and $\dot{R}$ is specified so far, we can postulate in addition

$$|\dot{R}| = (2H'')^{\frac{1}{2}}. \tag{4.4}$$

That is, we take $|\dot{R}|$ as the upper bound for the initial particle speed. [We assume that (3.1) is satisfied.] The induced electric field in $x > R$ is given by $\epsilon\dot{R}(B_2 - B_1)$.

Although for the Hamiltonian as given by (4.2) the equations of motion (2.11) can readily be solved in closed form for either half-space, the matching problem seems to make any explicit approach more complicated than the present one.

Looking at the assumptions listed in Sec. 2, we observe that (4.2) is of the form (2.1). We can identify

$$q_0(t) = \begin{cases} x_0 & \text{for } R \geq x_0 \\ R + (B_1/B_2)(x_0 - R) & \text{for } R < x_0. \end{cases} \tag{4.5}$$

The action integral J takes the form

$$J = \pi H\left(\frac{1}{B_1} + \frac{1}{B_2}\right) + 2H\left(\frac{1}{B_1} - \frac{1}{B_2}\right) \times [\arcsin\lambda + \lambda(1 - \lambda^2)^{\frac{1}{2}}], \quad -1 \leq \lambda \leq 1,$$
$$J = 2\pi H/B_2, \quad \lambda < 1$$
$$J = 2\pi H/B_1, \quad \lambda > 1, \quad \lambda = B_1(R - x_0)/(2H)^{\frac{1}{2}}. \tag{4.6}$$

For $\lambda^2 > 1$, the particle is separated, and for $\lambda^2 < 1$ it is connected to the front. Since with (2.5) and with $B_{\mathrm{I}} = \min(B_1, B_2)$, $B_{\mathrm{II}} = \max(B_1, B_2)$

$$\frac{2\pi H}{B_{\mathrm{II}}} \leq f(H, t) \leq \frac{2\pi H}{B_{\mathrm{I}}} \tag{4.7}$$

holds, we can choose in view of (2.7)

$$J' = \frac{2\pi H'}{B_{\mathrm{II}}}, \qquad J'' = \frac{2\pi H''}{B_{\mathrm{I}}},$$
$$H_0 = \frac{H'B_{\mathrm{I}}}{2B_{\mathrm{II}}}, \qquad H_1 = \frac{2H''B_{\mathrm{II}}}{B_{\mathrm{I}}}. \tag{4.8}$$

The assumptions of Sec. 2 concerning continuity and boundedness of $\psi(q, t)$ and $R(t)$ are clearly satisfied.

Thus (3.2) holds, and J is an adiabatic invariant. Using this we shall prove (i) indirectly, assuming that the particle passes through the front at time t'_{II} with θ being arbitrarily large, which then leads to a contradiction.

With the aid of (3.2) and (4.7) we can estimate

$$H(t_{\mathrm{II}}) < (B_{\mathrm{II}}/2\pi)(M_1\epsilon^{\frac{1}{2}}\theta + M_2\epsilon) + (B_{\mathrm{II}}/B_{\mathrm{I}})H(t_{\mathrm{I}}). \tag{4.9}$$

On the other hand, (4.2) immediately leads to a lower bound:

$$H(t_{\mathrm{II}}) \geq \tfrac{1}{2}B'^2[R(t_{\mathrm{II}}) - x_0]^2 \geq \tfrac{1}{2}B'^2[|\dot{R}|\,\epsilon\theta - |R(t_{\mathrm{I}}) - x_0|]^2. \tag{4.10}$$

It is clear that (4.9) and (4.10) cannot be satisfied for arbitrarily large θ. An upper limit θ^* is obtained by equating the right-hand sides of both estimates, which leads to

$$\theta^* = \frac{|R(t_{\mathrm{I}}) - x_0|}{\epsilon\,|\dot{R}|}[1 + O(\epsilon^{\frac{1}{2}})] + \frac{1}{\epsilon\,|\dot{R}|}\left(\frac{2B_{\mathrm{II}}H(t_{\mathrm{I}})}{B_{\mathrm{I}}^3}\right)^{\frac{1}{2}}[1 + O(\epsilon^{\frac{1}{2}})].$$

For sufficiently small ϵ we can write

$$\theta^* \leq \frac{2[2H(t_I)]^{\frac{1}{2}}}{|c|\,B_I}\left(1+\left(\frac{B_{II}}{2B_I}\right)^{\frac{1}{2}}\right) = \frac{N}{|c|}.$$

So, for $\theta > N/|c|$ there is a contradiction and the particle cannot move through the front again, which proves (i).

As for (ii), we first assume that the particle for $t' < \tau_I$ circles in $x < R$ which implies $R < 0$ because otherwise it never would touch the front.

By using (i) we immediately see that the particle has again to be separated from the front at any time $t' > \tau_I + N/|c|$ hitting the front for the last time at $t' = \tau_{II}$. It cannot have returned to $x < R$ because it would be met again by the front. So, it must be drifting on the other side and stay so because the front moves off with speed $\dot{R}$ while the drift speed is $\dot{R}(1 - B_1/B_2)$. The invariant for the initial and the final separated state is proportional to the magnetic moment H/B, as follows from (4.6) with $\lambda^2 > 1$. It is easy to see from the solutions of the equations of motion that H, and hence J, remain constant in the circling state and vary periodically with time in the drift state, the variation being of order ϵ.

According to (i), $\tau_{II} - \tau_I$ is of order $1/\epsilon$. Thus we see from (3.2) that the corresponding change of J is of order $\epsilon^{\frac{1}{2}}$ or smaller [according to the present notation we have $t_2 - t_1 = \epsilon(\tau_{II} - \tau_I) = 0(1)$]. Thus the entire change of J is of order $\epsilon^{\frac{1}{2}}$ which gives the result of point (ii).

If the particle initially drifts in $x < R$ (with $R > 0$), a suitable coordinate transformation leads to the situation just considered. It is easy to show that the corresponding change of J is of order ϵ so that the present results still hold. Similarly, (ii) holds if the magnetic moment for the final state is evaluated in the frame moving with the drift velocity.

Transforming to a frame of reference in which the front is at rest, we see from (4.3) and (4.4) that the variation of J is small if the drift velocity is small compared to the gyration speed. In an actual shock wave, this condition can, however, not be satisfied for all particles. In many cases of practical interest, however, the condition is fulfilled for (most of) the electrons and for the high-speed ions. Furthermore, the present results show that a plane discontinuity front cannot accelerate the fast particles to nonadiabatically high energies.[11]

ACKNOWLEDGMENT

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APPENDIX

Before estimating the integral

$$X = \int_{t_1}^{t_2} \left|\frac{\partial Y}{\partial t}\right| dt, \tag{A1}$$

with Y as defined in (3.25), we write down some properties needed later on.

Defining $F = Y^2 = H - \psi$ and noting that $|\dot{q}| = |p|/\epsilon \leq (2H_1)^{\frac{1}{2}}$, we can write for $(0, q)$ and $(0, R)$ in $Q''(t)$ and ϵ sufficiently small

$$\begin{aligned} |dF/dt| &= |\psi_t(q, t) - d\psi(R, t)/dt| < K_1\,, \\ |d^2F/dt^2| &= |\psi_{tt}(q, t) + \psi_{tq}(q, t)\dot{q} \\ &\quad - d^2\psi(R, t)/dt^2| < K_2/\epsilon, \end{aligned} \tag{A2}$$

where K_1, K_2, are constants, independent of ϵ. With

$$\tau = 2H_0^{\frac{1}{2}}/C, \qquad \delta = K_1\tau, \tag{A3}$$

where C is the upper bound on ψ_q for $(0, q)$ in $Q''(t)$ (see Assumption 5 in Sec. 2), we can establish the following property:

Consider a time interval $\Theta : [\tau', \tau' + \epsilon\tau]$ arbitrarily situated in $[t_1 - t_2]$ (ϵ is taken sufficiently small so that $\epsilon\tau$ is smaller than $t_2 - t_1$). Furthermore, consider an orbit staying in Q for t in $[t_2, t_1]$, on which during Θ

$$Y(t) \leq (2\epsilon\delta)^{\frac{1}{2}} \tag{A4}$$

is satisfied. Then, for sufficiently small ϵ there are not more than four points in Θ at which $q(t) - R(t)$ changes its sign (intersection points).

As a first step we shall show the following:

If an orbit stays in Q for a time interval during which $\ddot{q}$ is either always positive or negative, then for sufficiently small ϵ there are at most two intersections in that interval.

We first assume that in the interval considered, $\ddot{q}$ is positive. Since $\dot{q}$ and $\dot{R}$ are continuous, $\dot{q} - \dot{R}$ must either be zero or must have opposite signs at two successive intersections.

We assume that there is an intersection at $t = \tau_1$ with

$$\dot{q}(\tau_1) - \dot{R}(\tau_1) \geq 0. \tag{A5}$$

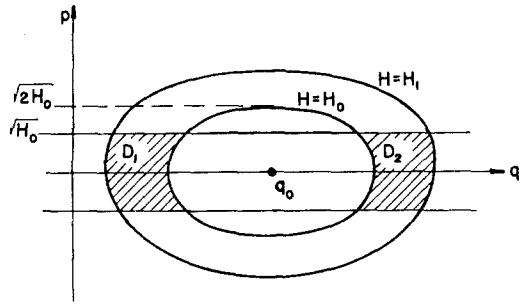

FIG. 3. The domain D, consisting of D_1 and D_2.

If such a point does not exist, there can only be one intersection and the claim holds trivially.

Now suppose in the interval considered there is another intersection with $t > \tau_1$; then there must be at least one, say at $t = \tau_2 > \tau_1$ where

$$\dot{q}(\tau_2) - \dot{R}(\tau_2) \leq 0 \tag{A6}$$

is satisfied. Denoting the lower bound of ψ_q in Q' by L and the upper bound of $\ddot{R}$ by A we can estimate

$$\dot{q}(\tau_1) + (L/\epsilon^2)(\tau_2 - \tau_1) - \dot{R}(\tau_1) - A(\tau_2 - \tau_1) < \dot{q}(\tau_2) - \dot{R}(\tau_2) \leq 0. \tag{A7}$$

For $\epsilon^2 < L/A$, (A7) contradicts (A5) so that the intersection at $t = \tau_2$ cannot exist. Since only one intersection is possible for $t < \tau_1$, we have the desired result. In the case $\ddot{q} < 0$ the proof is similar.

Now we are able to prove the property quoted above in the following way. Let D be the intersecting domain of $|p| \leq H_0^{\frac{1}{2}}$ and of Q. It consists of two separated, simply-connected domains D_1, D_2 lying in $q \gtrless q_0$, respectively (see Fig. 3). So, as follows from (2.3) and (2.9), ψ_q, $\dot{p}$, and $\ddot{q}$ have definite signs in D_1 and D_2.

At an intersection point we have $q = R$ and, therefore, from (2.1) and (3.25), $Y = |p|/2^{\frac{1}{2}}$ which, with the aid of (A3) and (A4), leads to

$$|p| \leq 2(\epsilon\delta)^{\frac{1}{2}} < H_0^{\frac{1}{2}} \quad \text{for} \quad \epsilon < H_0/4\delta, \tag{A8}$$

so that for sufficiently small ϵ the orbits considered here have all their intersection points lying in D. Now we consider that part of the orbit which, during Θ lies in D. It consists of a sequence of continuous sections which we denote by C_i. Since $\ddot{q}$ has a definite sign on every C_i, there are not more than two intersections on a given C_i.

We now estimate the time Δt necessary to cross the strip $|p| \leq H_0^{\frac{1}{2}}$. Since in D the function $p(t)$ varies monotonically with time, (2.9) yields

$$\Delta t = \left| \int_{-H_0^{\frac{1}{2}}}^{H_0^{\frac{1}{2}}} \frac{dp}{\dot{p}} \right| = \epsilon \int_{-H_0^{\frac{1}{2}}}^{H_0^{\frac{1}{2}}} \frac{dp}{|\psi_q|} > \epsilon \frac{2H_0^{\frac{1}{2}}}{C} = \epsilon\tau. \tag{A9}$$

As the interval Θ has the width $\epsilon\tau$ also, the orbit section associated with Θ can, at most, have two parts C_i and has therefore not more than four intersections, which completes the proof.

Now we note from (2.8) and (3.25) that for $(0, R)$ not in Q'', we have $Y \equiv 0$ so that, in view of (4.1), we can replace $\psi(R, t)$ by H_1 which also leads to $Y \equiv 0$ while now $(0, R)$ remains in Q''. So we need only consider $(0, R)$ in Q'' and we can use (A2).

Considering (A1), we divide the interval $[t_1, t_2]$ in subintervals L_i of width $\epsilon\tau$ and separate them into two classes:

M_i : containing at least one point $\bar{t}$ at which $Y(\bar{t}) > (2\epsilon\delta)^{\frac{1}{2}}$,

N_i : containing no such point.

For an arbitrary time t in an M interval we can write, using (3.25), (A2), and (A3),

$$|F(t)| = \left| F(\bar{t}) + \int_{\bar{t}}^{t} \dot{F}\, dt \right| > 2\epsilon\delta - \epsilon K_1 \tau = \epsilon\delta, \tag{A10}$$

so that

$$Y > (\epsilon\delta)^{\frac{1}{2}}. \tag{A11}$$

Using (2.9), it is easily shown that

$$\partial Y/\partial t = dY/dt, \tag{A12}$$

and we obtain from (A2) and (A12)

$$\left|\frac{\partial Y}{\partial t}\right| = \frac{1}{2Y}\left|\frac{dF}{dt}\right| < \frac{K_1}{2(\epsilon\delta)^{\frac{1}{2}}}. \tag{A13}$$

Therefore, the contribution of all M intervals to X can be estimated as

$$\sum_i \int_{M_i} \left|\frac{\partial Y}{\partial t}\right| dt < \frac{K_1}{2(\epsilon\delta)^{\frac{1}{2}}}(t_2 - t_1). \tag{A14}$$

In the N intervals, since we need continuity of $\dot{Y}$, we subdivide at every intersection point obtaining the subintervals N_i'. Since $Y \leq (2\epsilon\delta)^{\frac{1}{2}}$, there are not more than four intersections in one N interval so that the total number ν of N' intervals can be estimated by

$$\nu \leq 5[(t_2 - t_1)/\epsilon\tau + 1]. \tag{A15}$$

We split the N'-intervals further by all points at which $\dot{Y}$ changes its sign, obtaining the intervals N_i''. (For definiteness, we consider $\dot{Y} = 0$ positive.)

From the fact that in an N'' interval $\dot{Y}$ can only be discontinuous when $Y = 0$, it follows that $\dot{Y}$ vanishes at least at one boundary point with the possible exception of those N' intervals bounded by an intersection point (see Fig. 4). Ignoring these

exceptional cases for the moment, we can estimate with the aid of (A2),

$$|\dot{F}| < (K_2/\epsilon)\Delta\tau_i,$$

where $\Delta\tau_i$ denotes the width of the interval N_i''. Denoting the larger boundary value of F by F_L and the smaller one by F_S, we obtain

$$F_L - F_S < (K_2/\epsilon)(\Delta\tau_i)^2$$

and, therefore,

$$Y_L - Y_S < [(K_2/\epsilon)(\Delta\tau_i)^2 + Y_S^2]^{\frac{1}{2}} - Y_S \leq (K_2/\epsilon)^{\frac{1}{2}}\Delta\tau_i,$$

so that we now have the estimate (summed over one N' interval)

$$\sum_i \int_{N_i''} \left|\frac{\partial Y}{\partial t}\right| dt = \sum_i (Y_L - Y_S)_i < \left(\frac{K_2}{\epsilon}\right)^{\frac{1}{2}} \epsilon\tau + 2(2\epsilon\delta)^{\frac{1}{2}}, \quad \text{(A16)}$$

where the second term takes care of the exceptions mentioned above and is obtained in the following way: If an N'' interval does not have $\dot{Y} = 0$ at one endpoint (which is only possible if one endpoint is an intersection point) then Y must vanish at one endpoint. Furthermore, Y varies monotonically in every N'' interval. So, noting that $Y \leq (2\epsilon\delta)^{\frac{1}{2}}$ and using (A12), we can estimate (N_e'' denoting the exceptional time interval),

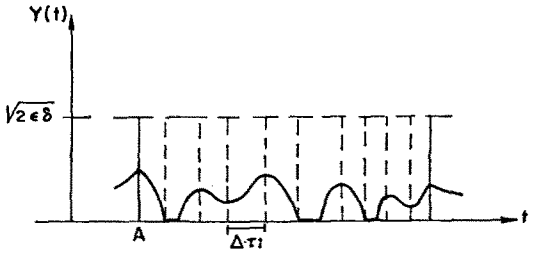

FIG. 4. Splitting of an N' interval into N'' intervals [the interval next to the intersection point A is of the exceptional type: $\dot{Y}(t)$ does not vanish at one boundary point].

$$\int_{N_e''} \left|\frac{\partial Y}{\partial t}\right| dt = \left|\int_{N_e''} \frac{dY}{dt}\, dt\right| \leq (2\epsilon\delta)^{\frac{1}{2}}.$$

As there are at most two such intervals in one N'-interval, their contribution to (A16) is smaller than or equal to $2(2\epsilon\delta)^{\frac{1}{2}}$. Since there are ν N'-intervals we finally obtain, observing (A15) and (A16) and including (A14):

$$X = \int_{t_1}^{t_2} \left|\frac{\partial Y}{\partial t}\right| dt < S_1\epsilon^{-\frac{1}{2}}(t_2 - t_1) + S_2\epsilon^{\frac{1}{2}},$$

where S_1 and S_2 are constants independent of ϵ. Thus, the estimate (A1) holds.

The Dirac Equation and the Unitary Representations of the Inhomogeneous Lorentz Group

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The Dirac equation in its quantized form is discussed in order to deduce the structure of the unitary representation of the Poincaré group in Fock space. There is a short account of discrete symmetries in Fock space and a simple method of calculating spin matrix elements is outlined.

I. INTRODUCTION

THE unitary representations of the inhomogeneous Lorentz group are well known, a complete classification of them was given already by Wigner in 1939.[1] Each irreducible representation is characterized by two quantum numbers, the mass and the spin. The solutions of the Dirac equation transform under the connected part of the homogeneous Lorentz group according to a four-dimensional spinor representation, which is reducible and not unitary. On second quantization one obtains a Hilbert space which is the direct sum of one, two, etc., particle subspaces, the so-called Fock representation. The transformation properties of the field define a unitary representation of the inhomogeneous Lorentz group in Fock space. This connection is implied in several places in the literature,[2] but to the author's knowledge it has not yet been spelled out in detail. The present paper intends to do this, hoping to combine clarity with simplicity by using elementary methods. There seem to be two considerations to justify this. If the notions of Hilbert space and relativistic invariance are pertinent to particle physics, the scattering processes are to be described by isometric wave operators which satisfy certain asymptotic conditions and establish a unitary equivalence between the "free" and "interacting" generators of the Poincaré group. One particular model for two spinless particles which satisfies all these conditions is already known.[3] For this kind of approach a detailed understanding of the Hilbert space spanned by the "free" states and the unitary representation of the Poincaré group on it, is essential. Secondly, the field equation supplies additional information with regard to symmetry, especially discrete symmetry. For example, the Dirac equation entails the existence of a pair of particles related through charge conjugation. There is nothing in the theory of the Poincaré group which necessitates this. Also, the Dirac equation limits the choices of possible time-reversal transformations.

The next introductory chapter contains a short discussion of the solutions of the Dirac equation, mainly in order to establish a unique phase convention for the spinors. (Normally helicity is used to classify further the positive and negative energy solutions, which still leaves the phases undermined). After this, the connection between the transformation properties of the field and the unitary representation in Fock space is explicitly demonstrated. This is followed by a short discussion of discrete symmetries; space, time inversion and charge conjugation. Finally, a method is briefly outlined by which matrix elements between spinors can be evaluated in a simple fashion.

2. SOLUTIONS OF THE DIRAC EQUATION

We start from the Dirac equation[4]

$$(-i\,\partial_\mu\gamma^\mu + m)\psi(x) = 0,$$

where $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$. A complete set of solutions is given by $u(p)e^{-ipx}$ and $v(p)e^{ipx}$, $p_0 > 0$, $p^2 = m^2$, where the four-component spinors satisfy

$$(-p_\mu\gamma^\mu + m)u(p) = 0, \tag{1}$$

$$(p_\mu\gamma^\mu + m)v(p) = 0. \tag{2}$$

For a given 4-vector p, there are two pairs of linearly independent solutions $u(p)$ and $v(p)$, provided $p^2 = m^2$. Normally one uses the helicity operator to distinguish further among these, but we employ a

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

[2] See, e.g., A. S. Wightman in *Dispersion Relations and Elementary Particles* (John Wiley & Sons, Inc., New York, 1960).

[3] T. F. Jordan, A. J. Macfarlane, and E. C. G. Sudarshan, Phys. Rev. 133, B487 (1964), and also L. B. Redei "Composite Particles in a Relativistic Model of Two-Body Scattering" (to be published).

[4] We shall be using the same conventions as in S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson and Company, Evanston, Illinois, 1961). In particular, $g^{00} = -g^{ii} = 1$, $g^{\alpha\beta} = 0$ if $\alpha \neq \beta$.

different set of solutions. Let $S(\Lambda)$ be the up-to-a-sign spinor representation of the homogeneous Lorentz group $\mathfrak{L}$ which satisfies[5]

$$S(\Lambda)^{-1}\gamma^{\mu}S(\Lambda) = \Lambda^{\mu}{}_{\nu}\gamma^{\nu}, \qquad \det S = 1, \tag{3}$$

for all $\Lambda \in \mathfrak{L}$. From Eqs. (1), (2), and (3) it follows that if $\Lambda p = q$, $\Lambda \in \mathfrak{L}$, then $S(\Lambda)u(p)$ is a $u(q)$ and also $S(\Lambda)v(p)$ is a $v(q)$. Following Wigner we define a set of transformations[1] $L(p)^{\mu}{}_{\nu}$,

$$L(p)^0{}_0 = m^{-1}p^0, \qquad L(p)^0{}_k = L(p)^k{}_0 = -m^{-1}p^k,$$
$$L(p)^k{}_l = \delta^k{}_l + [m(m + p^0)]^{-1}p^k p^l. \tag{4}$$

The L(p) have the properties

$$L(p) \in \mathfrak{L}, \qquad L(p)p = \bar{p} \quad \text{or} \quad L(p)^{-1}\bar{p} = p, \tag{5}$$

where $\bar{p} = (m, \mathbf{0})$. For simplicity we now choose a particular set of γ matrices:

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma^k = \begin{pmatrix} 0 & \sigma^k \\ -\sigma^k & 0 \end{pmatrix}, \tag{6}$$

where σ^k are the Pauli matrices.[4] (A different choice for the γ matrices would give a different but nevertheless equivalent representation in Fock space.) Let

$$u_1(\bar{p}) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad u_2(\bar{p}) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad v_1(\bar{p}) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},$$

and

$$v_2(\bar{p}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

We define $u_i(p)$ and $v_i(p)$, $i = 1, 2, \cdots$, by

$$u_i(p) = S[L(p)^{-1}]u_i(\bar{p}), \qquad v_i(p) = S[L(p)^{-1}]v_i(\bar{p}). \tag{7}$$

One might object that S being a double-valued representation, Eq. (7) determines $u_i(p)$ and $v_i(p)$ only up to a sign. However, Eq. (4) defines a continuous one $\leftrightarrow$ one mapping of the singly connected parameter domain $p^2 = m^2$, $p^0 > 0$, into $\mathfrak{L}$. The image set $L(p)$ is therefore singly connected. We can fix the sign uniquely by choosing $S[L(\bar{p})^{-1}] = I$. For any $\Lambda \in \mathfrak{L}$ and any 4-vector p, $p^2 = m^2$, $p^0 > 0$, we define[1]

$$Q(p, \Lambda) = L(p)\Lambda L(\Lambda^{-1}p)^{-1}. \tag{8}$$

Straightforward computation shows that

$$Q(p, \Lambda_1)Q(\Lambda_1^{-1}p, \Lambda_2) = Q(p, \Lambda_1\Lambda_2) \tag{9}$$

and also

$$Q(\bar{p}, \Lambda)\bar{p} = \bar{p},$$

i.e., the $Q(p, \Lambda)$ are pure rotations. For the representation S one has the corresponding equations:

$$S[Q(p, \Lambda)] = S[L(p)]S(\Lambda)S[L(\Lambda^{-1}p)^{-1}], \tag{10}$$

$$S[Q(p, \Lambda_1)]S[Q(\Lambda_1^{-1}p, \Lambda_2)] = \pm S[Q(p, \Lambda_1\Lambda_2)], \tag{11}$$

where in the last equation the choice of sign is made to correspond to the sign in the equation $S(\Lambda_1)S(\Lambda_2) = \pm S(\Lambda_1\Lambda_2)$. This can be best seen by considering $S(\Lambda)$ as being a single-valued representation of the covering group. The path associated with Λ in Eq. (10) then determines the path of $S[Q(p, \Lambda)]$ in such a way that Eq. (11) holds [see the remark after Eq. (7)]. The $S[Q(p, \Lambda)]$ have two important properties:

(a) They are unitary matrices. This follows from the fact that $S[Q(p, \Lambda)]$ maps the $u_i(\bar{p})$ and $v_i(\bar{p})$ into perpendicular unit vectors.[6]

(b) The spinor $S[Q(p, \Lambda)]u_i(\bar{p})$ is a $u(\bar{p})$ and similarly $S[Q(p, \Lambda)]v_i(\bar{p})$ is a $v(\bar{p})$. The matrices $S[Q(p, \Lambda)]$ thus decompose, which we write as

$$S[Q(p, \Lambda)] = D^u(p, \Lambda) \oplus D^v(p, \Lambda), \tag{12}$$

where $D^{u,v}(p, \Lambda)$ are 2×2 unitary matrices which, because of Eq. (11), satisfy

$$D^{u,v}(p, \Lambda_1)D^{u,v}(\Lambda_1^{-1}p, \Lambda_2) = \pm D^{u,v}(p, \Lambda_1\Lambda_2). \tag{13}$$

3. REPRESENTATION OF THE INHOMOGENEOUS LORENTZ GROUP IN FOCK SPACE

We write the four-component field operator $\psi(x)$ in the form

$$\psi(x) = (2\pi)^{-\frac{3}{2}} \int d^3p \left(\frac{m}{p^0}\right)^{\frac{1}{2}} \times \sum_i [u_i(p)e^{-ipx}c_i(p) + v_i(p)e^{ipx}\, d_i^{\dagger}(p)], \tag{14}$$

where c_i and d_i are the usual annihilation operators:

$$[c_i(p), c_j^{\dagger}(p')]_+ = [d_i(p), d_j^{\dagger}(p)]_+ = \delta_{ij}\delta(\mathbf{p} - \mathbf{p}').$$

The transformation law[4]

$$U(\Lambda, a)^{-1}\psi_{\alpha}(x)U(\Lambda, a) = \sum_{\beta} S(\Lambda)_{\alpha\beta}\psi_{\beta}(\Lambda^{-1}(x - a)) \tag{15}$$

defines a representation of the Poincaré group $\{\Lambda, a\}$. First we determine how they act on the creation operators $c_i^{\dagger}(p)$ and $d_i^{\dagger}(p)$. From Eqs. (14) and (15)

[5] See e. g., H. Boerner, *Representations of Groups* (John Wiley & Sons, Inc., New York, 1963).

[6] For the proof of this, one has to use that for Hermitian γ^0, $S^{+}\gamma^0 = \gamma^0 S^{-1}$, see e.g., Schweber, Ref. 4.

$$U(\Lambda, a)^{-1}\psi(x)U(\Lambda, a)$$
$$= (2\pi)^{-\frac{3}{2}} \int d^3p \left(\frac{m}{p^0}\right)^{\frac{1}{2}} \sum_i [S(\Lambda)u_i(p)e^{-ip[\Lambda^{-1}(x-a)]}c_i(p)$$
$$+ S(\Lambda)v_i(p)e^{ip[\Lambda^{-1}(x-a)]}\, d_i^\dagger(p)]$$
$$= (2\pi)^{-\frac{3}{2}} \int d^3p \left(\frac{m}{p^0}\right)^{\frac{1}{2}} \left(\frac{(\Lambda^{-1}p)^0}{p^0}\right)^{\frac{1}{2}}$$
$$\times \sum_i [S(\Lambda)u_i(\Lambda^{-1}p)e^{ipa}e^{-ipx}c_i(\Lambda^{-1}p)$$
$$+ S(\Lambda)v_i(\Lambda^{-1}p)e^{-ipa}e^{ipx}\, d_i^\dagger(\Lambda^{-1}p)]. \quad (16)$$

Now we use Eq. (10) to express $S(\Lambda)$ in terms of $S[Q(p, \Lambda)]$ and $S[L(p)]$:

$$S(\Lambda) = S[L(p)^{-1}]S[Q(p, \Lambda)]S[L(\Lambda^{-1}p)].$$

Substitution into Eq. (16), together with Eqs. (7) and (13), gives

$$U(\Lambda, a)^{-1}\psi(x)U(\Lambda, a)$$
$$= (2\pi)^{-\frac{3}{2}} \int d^3p \left(\frac{m}{p^0}\right)^{\frac{1}{2}} \left(\frac{(\Lambda^{-1}p)^0}{p^0}\right)^{\frac{1}{2}} \sum_i S[L(p)^{-1}]$$
$$\times [D^u(p, \Lambda)u_i(\tilde{p})e^{ipa}e^{-ipx}c_i(\Lambda^{-1}p)$$
$$+ D^v(p, \Lambda)v_i(\tilde{p})e^{-ipa}e^{ipx}\, d_i^\dagger(\Lambda^{-1}p)],$$

and finally

$$U(\Lambda, a)^{-1}\psi(x)U(\Lambda, a) = (2\pi)^{-\frac{3}{2}} \int d^3p \left(\frac{m}{p^0}\right)^{\frac{1}{2}} \left(\frac{(\Lambda^{-1}p)^0}{p^0}\right)^{\frac{1}{2}}$$
$$\times \sum_{i,j} [D^u_{ji}(p, \Lambda)u_j(p)e^{ipa}e^{-ipx}c_i(\Lambda^{-1}p)$$
$$+ D^v_{ji}(p, \Lambda)v_j(p)e^{-ipa}e^{ipx}\, d_i^\dagger(\Lambda^{-1}p)].$$

On the other hand,

$$U(\Lambda, a)^{-1}\psi(x)U(\Lambda, a) = (2\pi)^{-\frac{3}{2}} \int d^3p \left(\frac{m}{p^0}\right)^{\frac{1}{2}}$$
$$\times \sum_i [u_i(p)e^{-ipx}U(\Lambda, a)^{-1}c_i(p)U(\Lambda, a)$$
$$+ v_i(p)e^{ipx}U(\Lambda, a)^{-1}\, d_i^\dagger(p)U(\Lambda, a)].$$

Comparing this with the previous equation one obtains

$$U(\Lambda, a)^{-1}c_i(p)U(\Lambda, a)$$
$$= \sum_j [(\Lambda^{-1}p)^0/p^0]^{\frac{1}{2}}e^{ipa}D^u_{ij}(p, \Lambda)c_j(\Lambda^{-1}p), \quad (17)$$

$$U(\Lambda, a)^{-1}\, d_i^\dagger(p)U(\Lambda, a)$$
$$= \sum_j [(\Lambda^{-1}p)^0/p^0]^{\frac{1}{2}}e^{-ipa}D^v_{ij}(p, \Lambda)\, d_j^\dagger(\Lambda^{-1}p) \quad (18)$$

or

$$U(\Lambda, a)c_i^\dagger(p)U(\Lambda, a)^{-1}$$
$$= [(\Lambda p)^0/p^0]^{\frac{1}{2}}e^{i\Lambda p\cdot a} \sum_j D^u_{ji}(\Lambda p, \Lambda)c_j^\dagger(\Lambda p), \quad (19)$$

$$U(\Lambda, a)\, d_i^\dagger(p)U(\Lambda, a)^{-1}$$
$$= [(\Lambda p)^0/p^0]^{\frac{1}{2}}e^{i\Lambda p\cdot a} \sum_j D^{v*}_{ji}(\Lambda p, \Lambda)\, d_j^\dagger(\Lambda p), \quad (20)$$

where the asterisk * denotes complex conjugation. The particle space H is an infinite direct sum of subspaces

$$H = \sum_{n,m} \oplus H^{n,m},$$

where the $H^{n,m}$ consist of vectors of the form

$$f^{n,m} \sim (n!)^{-\frac{1}{2}}(m!)^{-\frac{1}{2}}$$
$$\times \int \frac{d^3p_1}{(p_1^0)^{\frac{1}{2}}} \cdots \int \frac{d^3p_n}{(p_n^0)^{\frac{1}{2}}} \int \frac{d^3q_1}{(q_1^0)^{\frac{1}{2}}} \cdots \int \frac{d^3q_m}{(q_m^0)^{\frac{1}{2}}}$$
$$\times \sum_i \sum_j c_{i_1}^\dagger(p_1) \cdots c_{i_n}^\dagger(p_n)d_{j_1}^\dagger(q_1) \cdots d_{j_m}^\dagger(q_m)$$
$$\times f^{n,m}(p_1, \cdots p_n; q_1, \cdots q_m)_{i_1,\cdots i_n;j_1\cdots j_m} |0\rangle \quad (21)$$

with the restriction that the functions $f^{n,m}$ are antisymmetric in the first n and the last m spin and momentum variables. The inner product is given by

$$(f^{n,m}, g^{n',m'}) = \delta_{nn'}\delta_{mm'}$$
$$\times \int \frac{d^3p_1}{(p_1^0)} \cdots \int \frac{d^3p_n}{(p_n^0)} \int \frac{d^3q_1}{(q_1^0)} \cdots \int \frac{d^3q_m}{(q_m^0)}$$
$$\times \sum_i \sum_j f^{n,m*}(p_1, \cdots p_n; q_1, \cdots q_m)_{i_1\cdots i_n;j_1\cdots j_m}$$
$$\times g^{n',m'}(p_1, \cdots p_n; q_1, \cdots q_m)_{i_1,\cdots i_n;j_1,\cdots j_m}. \quad (21')$$

The transformation laws (19) and (20) imply, assuming the vacuum state to be invariant,

$$[U(\Lambda, a)f^{1,0}](p)_r = e^{ipa} \sum_s D^u_{rs}(p, \Lambda)f^{1,0}(\Lambda^{-1}p)_s, \quad (22)$$

$$[U(\Lambda, a)f^{0,1}](p)_r = e^{ipa} \sum_s D^{v*}_{rs}(p, \Lambda)f^{0,1}(\Lambda^{-1}p)_s. \quad (23)$$

The transformation law in the many-particle spaces $H^{n,m}$ is obtained simply by taking tensor products of $H^{1,0}$ and $H^{0,1}$. The transformations (22) and (23) are indeed unitary with respect to the inner product (21′) and taken together with Eq. (13) they define a pair of irreducible representations[2] of the inhomogeneous Lorentz group. The other subspaces obtained by taking tensor products are invariant but no longer irreducible.

We now discuss briefly the infinitesimal generators. In view of the remark above we can restrict ourselves to $H^{1,0}$ and $H^{0,1}$. The generators of the subgroup of translations $U(1, a)$ are the multiplications by p^μ. To obtain the other generators $\mathbf{J}$ and $\mathbf{N}$ we have to use the formula

$$S[\Lambda(\lambda)] = I + \tfrac{1}{8}\lambda^{\mu\nu}(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu) \quad (24)$$

for an infinitesimal Lorentz transformation $\Lambda^\mu{}_\nu =$

$\delta^\mu{}_\nu + \lambda^\mu{}_\nu$. This is proved, e.g., in Ref. (4). The generator $\mathbf{J}$ is defined by

$$U[\Lambda(\theta)] = I - i\theta\mathbf{n}\cdot\mathbf{J},$$

for $\Lambda(\theta)^\mu{}_\nu = \delta^\mu{}_\nu + \lambda^\mu{}_\nu$, where

$$\lambda^{0\alpha} = \lambda^{\alpha 0} = 0, \qquad \lambda^{kl} = \theta\epsilon^{klm}n^m,$$

and θ is small. Equations (4) and (8) allow one to calculate $Q[p, \Lambda(\theta)]$;

$$Q[p, \Lambda(\theta)]^{\mu\nu} = g^{\mu\nu} + \lambda^{\mu\nu},$$

which, with our particular choice of the γ matrices, gives

$$S\{Q[p, \Lambda(\theta)]\} = I - i\theta\mathbf{n}\cdot(\mathbf{\Sigma} \oplus \mathbf{\Sigma}),$$

where $\mathbf{\Sigma} = \frac{1}{2}\boldsymbol{\sigma}$. Combining this with Eqs. (22) and (23) we have

$$\begin{aligned}(\mathbf{J}f^{1,0})(p)_r &= -i\mathbf{p} \wedge \partial f^{1,0}(p)_r + \sum_q \mathbf{s}^u_{rq} f^{1,0}(p)_q,\\ (\mathbf{J}f^{0,1})(p)_r &= -i\mathbf{p} \wedge \partial f^{0,1}(p)_r + \sum_q \mathbf{s}^v_{rq} f^{0,1}(p)_q,\end{aligned} \tag{25}$$

where

$$\mathbf{s}^u = \mathbf{\Sigma} \quad \text{and} \quad \mathbf{s}^v = -\mathbf{s}^{u*}. \tag{26}$$

This shows that $D^v(p, \Lambda) = D^u(p, \Lambda)^*$.

Similarly, $\mathbf{N}$ is defined by

$$U[\Lambda(\theta)] = I - i\theta\mathbf{n}\cdot\mathbf{N}$$

for $\Lambda(\theta)^\mu{}_\nu = \delta^\mu{}_\nu + \lambda^\mu{}_\nu$, where $\lambda^{00} = \lambda^{kl} = 0$ and $\lambda^{k0} = \lambda^{0k} = \theta n^k$. In this case one has

$$Q[p, \Lambda(\theta)]^\mu{}_\nu = \delta^\mu{}_\nu + \Delta Q[p, \Lambda(\theta)]^\mu{}_\nu,$$

where $\Delta Q^{0\alpha} = \Delta Q^{\alpha 0} = 0$ and

$$\Delta Q^{kl} = \theta(m + p^0)^{-1}(p^k n^l - p^l n^k)$$

giving

$$S\{[Q(p, \Lambda(\theta)]\} = I + i\theta(m + p^0)^{-1}\mathbf{n}\cdot[\mathbf{p} \wedge (\mathbf{\Sigma} \oplus \mathbf{\Sigma})],$$

and finally

$$\begin{aligned}(\mathbf{N}f^{1,0})(p)_r &= -ip^0\,\partial f^{1,0}(p)_r\\ &\quad - (m + p^0)^{-1}\sum_q \mathbf{p} \wedge \mathbf{s}^u_{rq} f^{1,0}(p)_q,\\ (\mathbf{N}f^{0,1})(p)_r &= -ip^0\,\partial f^{0,1}(p)_r\\ &\quad - (m + p^0)^{-1}\sum_q \mathbf{p} \wedge \mathbf{s}^v_{rq} f^{0,1}(p)_q.\end{aligned} \tag{27}$$

This concludes the discussion of the connected part of the inhomogeneous Lorentz group. The next chapter contains a short account of the discrete symmetries.

4. DISCRETE SYMMETRIES. CALCULATION OF MATRIX ELEMENTS

For the sake of completeness we now discuss parity, time reversal, and charge conjugation. In this connection see Ref. 6.

a. Parity

This is given by a unitary transformation $U(i_s)$ which satisfies $U(i_s)^2 = \pm 1$. It acts on the field $\psi(x)$ according to

$$\begin{aligned}U(i_s)^{-1}\psi(x)U(i_s) &= n_p(2\pi)^{-\frac{3}{2}}\int d^3p\,(m/p^0)^{\frac{1}{2}}\\ &\times \sum_i [\gamma^0 u_i(-\mathbf{p})e^{-ipx}c_i(-\mathbf{p}) + \gamma^0 v_i(-\mathbf{p})e^{ipx}\,d_i^\dagger(-\mathbf{p})]\\ &= n_p(2\pi)^{-\frac{3}{2}}\int d^3p\,(m/p^0)^{\frac{1}{2}}\sum_i \{\gamma^0 S[L(-\mathbf{p})^{-1}]\\ &\times u_i(\tilde{p})e^{-ipx}c_i(-\mathbf{p}) + \gamma^0 S[L(-\mathbf{p})^{-1}]v_i(\tilde{\mathbf{p}})e^{ipx}\,d_i^\dagger(-\mathbf{p})\},\end{aligned}$$

where $(n_P)^2 = \pm 1$. From Eqs. (3) and (4) follows

$$\begin{aligned}&\gamma^0 S[L(-\mathbf{p})^{-1}]^{-1}\gamma^0\gamma^\mu\gamma^0 S[L(-\mathbf{p})^{-1}]\gamma^0\\ &\qquad = [L(\mathbf{p})^{-1}]^\mu{}_\nu\gamma^\nu = S[L(\mathbf{p})^{-1}]^{-1}\gamma^\mu S[L(\mathbf{p})^{-1}]\end{aligned}$$

implying

$$S[L(\mathbf{p})^{-1}]\gamma^0 S[L(-\mathbf{p})^{-1}]^{-1}\gamma^0 = I.$$

{Here we made use of the irreducibility of γ^u and the convention $S[L(\tilde{p})^{-1}] = I$.} This gives

$$\begin{aligned}U(i_s)^{-1}\psi(x)U(i_s) &= n_p(2\pi)^{-\frac{3}{2}}\int d^3p\left(\frac{m}{p^0}\right)^{\frac{1}{2}}\\ &\times \sum_i [u_i(p)e^{-ipx}c_i(-\mathbf{p}) - v_i(p)e^{ipx}\,d_i^\dagger(-\mathbf{p})]\end{aligned}$$

or

$$\begin{aligned}U(i_s)^{-1}c_i(\mathbf{p})U(i_s) &= n_p c_i(-\mathbf{p}),\\ U(i_s)^{-1}d_i^\dagger(\mathbf{p})U(i_s) &= -n_p d_i^\dagger(-\mathbf{p}),\end{aligned}$$

and finally

$$\begin{aligned}[U(i_s)f^{1,0}](\mathbf{p})_r &= n_p f^{1,0}(-\mathbf{p})_r,\\ [U(i_s)f^{0,1}](\mathbf{p})_r &= -n_p^* f^{0,1}(-\mathbf{p})_r.\end{aligned} \tag{28}$$

b. Time Reversal

Time reversal is an antiunitary transformation $U(i_t)$ defined by

$$U(i_t)^{-1}\psi(x)U(i_t) = T\psi(-t, x), \tag{29}$$

where the matrix T satisfies

$$T^{-1}\gamma^{0*}T = \gamma^0, \qquad T^{-1}\gamma^{k*}T = -\gamma^k.$$

With our choice for the γ matrices

$$T = n_T\gamma^5\gamma^2\gamma^0, \qquad |n_T| = 1.$$

Writing down Eq. (29) in detail one has

$$U(i_t)^{-1}\psi(x)U(i_t) = n_T(2\pi)^{-\frac{3}{2}}\int d^3p\left(\frac{m}{p^0}\right)^{\frac{1}{2}} \times \sum_i [\gamma^5\gamma^2\gamma^0 u_i(-\mathbf{p})e^{ipx}c_i(-\mathbf{p}) + \gamma^5\gamma^2\gamma^0 v_i(-\mathbf{p})e^{-ipx}d_i^\dagger(-\mathbf{p})].$$

Using the elementary relations

$$\begin{aligned}\gamma^0 S[L(-\mathbf{p})^{-1}] &= S[L(\mathbf{p}^{-1})]\gamma^0,\\ \gamma^5 S[L(p)^{-1}] &= -S[L(p)^{-1}]\gamma^5,\\ \gamma^2 S[L(p)^{-1}] &= S[L(p)^{-1}]^*\gamma^5,\end{aligned} \tag{30}$$

one obtains the equations

$$\begin{aligned}U(i_t)^{-1}c_r(\mathbf{p})U(i_t) &= n_T(-1)^r c_{r+1}(-\mathbf{p}) \pmod 2,\\ U(i_t)^{-1}d_r^\dagger(\mathbf{p})U(i_t) &= n_T(-1)^r d_{r+1}^\dagger(-\mathbf{p}) \pmod 2.\end{aligned} \tag{31}$$

In the derivation it is important to remember that $U(i_t)$ is antiunitary, i.e.,

$$U(i_t)^{-1}\psi(x)U(i_t) = (2\pi)^{-\frac{3}{2}}\int d^3p\left(\frac{m}{p^0}\right)^{\frac{1}{2}} \times \sum_r [u_r^*(p)e^{ipx}U(i_t)^{-1}c_r(p)U(i_t) + v_r^*(p)e^{-ipx}U(i_t)^{-1}d_r^\dagger(p)U(i_t)].$$

Equation (31) leads to the transformation law in Fock space

$$\begin{aligned}[U(i_t)f^{1,0}](\mathbf{p})_r &= n_T^*(-1)^r f^{1,0*}(-\mathbf{p})_{r+1} \pmod 2,\\ [U(i_t)f^{0,1}](\mathbf{p})_r &= n_T(-1)^r f^{0,1*}(-\mathbf{p})_{r+1} \pmod 2.\end{aligned}$$

Notice that always $U(i_t)^2 = -I$.

c. Charge Conjugation

This is given by the unitary transformation C,

$$C\psi(x)C^{-1} = A\gamma^{0T}\psi^\dagger(x),$$

where ^{T} denotes the transposed matrix and A satisfies

$$A^{-1}\gamma^\mu A = -\gamma^{\mu T}.$$

In our case $A = n_C\gamma^2\gamma^0$, $|n_C| = 1$. An argument completely analogous to the one used in the two previous cases gives the final result

$$\begin{aligned}(Cf^{1,0})(p)_r &= -in_c^*(-1)^{r+1}f^{0,1}(p)_{r+1} \pmod 2,\\ (Cf^{0,1})(p)_r &= in_c(-1)^r f^{1,0}(p)_{r+1}. \pmod 2.\end{aligned} \tag{33}$$

At first sight, one might think that Eq. (33) implies changing the z component of the spin on charge conjugation. This is not so. The spin generators $\mathbf{s}^u$ and $\mathbf{s}^v$ in the two subspaces are not the same, they are related through Eq. (26).

Matrix elements of the type $\bar{u}_i(p)\Gamma u_j(p)$, where Γ is some linear combination of the sixteen independent products of γ matrices, can easily be evaluated. By means of the relation $S^+(\Lambda)\gamma^0 = \gamma^0 S(\Lambda)^{-1}$ and Eqs. (3), (4), and (7) they can be put into the form $u_i(p)\Gamma'(p)u_j(p)$ where $\Gamma'(p)$ is again a linear combination of products of γ matrices, the coefficients being functions of p. The terms which contain an odd number of γ^k, $k = 1, 2, 3$, do not contribute and one merely has to take the i, j element of the remaining terms which can contain γ^0 or $\gamma^k\gamma^l$. Sums of the form $\sum_i \bar{u}_i(p)\Gamma u_i(p)$ are even simpler as γ^0 is the only γ matrix whose trace over the upper left block does not vanish. The same is true for matrix elements which involve the spinors $v_i(p)$.

The solutions $u_i(p)$ and $v_i(p)$ used in this paper are the center-of-mass spin eigenfunctions. They are related to the more customary eigenspinors of the helicity operator $h(p) = i\,|\mathbf{p}|^{-1}\,\gamma^0\gamma^5\boldsymbol{\gamma}\cdot\mathbf{p}$ in the following way: first of all

$$[h(p), \gamma^0] = 0,$$

and so one can solve the eigenvalue equation

$$h(p)\sum_i a_\pm(p)_i u_i(\bar{p}) = \pm\sum_i a_\pm(p)_i u_i(\bar{p}),$$

where the coefficients $a_\pm(p)_i$ depend on p. In addition, using Eqs. (3) and (4) one verifies

$$[S(L(p)^{-1}), h(p)] = 0,$$

implying that the spinors $u_\pm(p) = \sum_i a_\pm(p)_i u_i(p)$ satisfy both

$$(-p_\mu\gamma^\mu + m)u_\pm(p) = 0$$

and

$$h(p)u_\pm(p) = \pm u_\pm(p).$$

The same procedure applies to the spinors $v(p)$.

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