Summation of Perturbation Series in Quantum Mechanics

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This is the first in a series of papers. It deals with the linked-cluster summation of the perturbation series in quantum mechanics and quantum statistical physics. In particular, a formalism is developed for calculating the matrix element of the operator $\exp(+sH)$, where H is the quantum-mechanical Hamiltonian operator. It is found that the matrix element may be written as an ordinary c-number integral of a c-number function over the phase space. This function is found by doing a linked-cluster summation of the usual perturbation series. It is in the form of an exponential of an effective Hamiltonian, H_{eff}, which is a function of the parameter s and the c-number momentum and position coordinates. We have assumed that the Hamiltonian has no spin-dependent terms. The matrix element is written in such a form that it may be used for calculating the transition matrix elements in time-dependent perturbation theory as well as for calculating the canonical partition function Z_N in quantum statistical mechanics. The former is obtained by substituting $s=-it/\hbar$ and the latter by substituting $s=-\beta$. The series for H_{eff} depends only on the potential and is independent of the statistics. The effects of the statistics (Bose-Einstein, Fermi-Dirac, or Maxwell-Boltzmann) are all included in a certain factor multiplying $\exp(sH_{\text{eff}})$. Thus we have succeeded in separating the statistical and quantum corrections. These latter arise from the noncommutativity of the position and momentum operators. The effective Hamiltonian is an infinite series. A diagrammatic technique is given for evaluating this series. It is an expansion in powers of the coupling constant and can also be expanded in powers of Planck's constant. In general, it is not possible to give a closed-form expression for H_{eff}. But for most practical cases it is sufficient to keep the first few powers of Planck's constant $\hbar$, because it is very small. We therefore have an entirely new method of approximation. The statistical effect may always be included exactly. No numerical estimates are made in this paper.

I. INTRODUCTION

The purpose of this work is to develop a method which will yield a linked-cluster sum for the matrix element of the operator $\exp(s\underline{H})$, where $\underline{H}$ is the Hamiltonian.[1] We use plane-wave states (eigenstates of the momentum operator). The matrix element is written as

$$M(s,\vec{\mathrm{p}}',\vec{\mathrm{p}})\equiv\langle\vec{\mathrm{p}}'|\exp(s\underline{H})|\vec{\mathrm{p}}\rangle\,. \tag{1.1}$$

Here $|\vec{\mathrm{p}}'\rangle$ and $|\vec{\mathrm{p}}\rangle$ are the momentum eigenstates.

We assume that the Hamiltonian is

$$\underline{H}\equiv\underline{K}(\vec{\underline{\mathrm{p}}})+V(\vec{\mathrm{r}})\,. \tag{1.2}$$

Here

$$\underline{K}(\vec{\underline{\mathrm{p}}})\equiv\sum_{\alpha=1}^{N}(\vec{\underline{\mathrm{p}}}_\alpha)^2/2m,$$

$$V\equiv V(\vec{\mathrm{r}})\equiv V(\vec{\mathrm{r}}_1,\vec{\mathrm{r}}_2,\ldots,\vec{\mathrm{r}}_N)\,. \tag{1.3}$$

The Hamiltonian $\underline{H}'$,

$$\underline{H}'=\sum_{\alpha=1}^{N}(\vec{\underline{\mathrm{p}}}_\alpha)^2/2m+\sum_{\alpha=1}^{N}[\vec{\nabla}V_1^{(\alpha)}\cdot\vec{\underline{\mathrm{p}}}_\alpha+\vec{\underline{\mathrm{p}}}_\alpha\cdot\vec{\nabla}V_1^{(\alpha)}]+V_0\,,$$

may easily be written in the form (1.2) by making the transformation

$$\vec{\underline{\mathrm{p}}}'_\alpha=\vec{\underline{\mathrm{p}}}_\alpha+2m\vec{\nabla}V_1^{(\alpha)},$$

$$V'=V_0(\vec{\mathrm{r}})-\sum_{\alpha=1}^{N}2m(\vec{\nabla}V_1^{(\alpha)})^2$$

In Eq. (1.1) there is no restriction on the potential except that it leads to a finite value for the partition function. Also we specifically assume that the Hamiltonian is spin-independent. An entirely different type of analysis is required for the latter type of interaction.

It is found that M in Eq. (1.1) may be written as

$$M(s,\vec{\mathrm{p}}',\vec{\mathrm{p}})=\int\prod_{\alpha=1}^{N}d^3p_\alpha d^3r_\alpha\psi^*_{\vec{\mathrm{p}}'}(r)\psi_{\vec{\mathrm{p}}}(\vec{\mathrm{r}})\times\exp\{s[E(\vec{\mathrm{p}}'_\alpha,\vec{\mathrm{r}}_\alpha)+\overline{V}(s,\vec{\mathrm{r}}_\alpha,\vec{\mathrm{p}}_\alpha)]\}\,.$$

Here E is the classical energy and $\overline{V}$ is a c-number function of s, $\vec{\mathrm{r}}$, and $\vec{\mathrm{p}}$. Also $\psi_{\vec{\mathrm{p}}}(\vec{\mathrm{r}})$ represents the properly symmetrized plane-wave eigenfunction.

In order to evaluate the transition amplitude we put

$$s=-it/\hbar. \tag{1.4}$$

This will give us the amplitude that the state $|\vec{\mathrm{p}}\rangle$ scatters into the state $|\vec{\mathrm{p}}'\rangle$ after a time t.

Similarly, if we put

$$s=-\beta,\quad \vec{p}'=\vec{p} \tag{1.5}$$

and then integrate over $\vec{p}$, we shall get the partition function Z_N for N particles:

$$Z_N=\mathrm{Tr}[\exp(-\beta_m H)]\,.$$

Hence,

$$Z_N=\int d^3p\,d^3r\,\exp[-\beta H_{\mathrm{eff}}(-\beta,\vec{r},\vec{p})]\,|\psi_{\vec{p}}^{\pm}(\vec{r})|^2\,. \tag{1.6}$$

Here,

$$\int d^3p\,d^3r\equiv\int\prod_{\alpha=1}^{N}d^3p_\alpha d^3r_\alpha\,. \tag{1.7}$$

The formula (1.6) is very interesting. We find that the quantum partition function Z_N is equivalent to the classical partition function with a different effective Hamiltonian independently of the statistics and a phase-space density $|\psi_{\vec{p}}^{\pm}(\vec{r})|^2$ which depends only on the statistics. This result has very interesting theoretical significance.

The outline of the paper is as follows. In Sec. II the problem is formulated. The method for calculating the effective Hamiltonian by doing a linked-cluster sum is given in Sec. III. The results are discussed in Sec. IV. Finally a brief summary and some interesting conclusions are given in Sec. V. An Appendix is added in which the details are given.

II. FORMULATION OF THE PROBLEM

The fundamental problem in quantum mechanics is to find the eigenvalues of a Hamiltonian. In general, this cannot be done exactly. In most cases we have to develop a method of self-consistent approximations. The approximation method usually employed is a development of the eigenvalues and eigenfunctions in powers of the coupling constant. This is a good approximation only if the coupling constant is not very large. In this section we formulate the problem in such a way as to yield a new method of approximation.

We consider a Hamiltonian H, of N identical particles. Only the nonrelativistic problem is considered in this paper. Also, we are considering particles of spin zero. This is to simplify the algebra. The Hamiltonian is assumed to be

$$\underline{H}\equiv\underline{K}(\underline{\vec{p}})+V(\vec{r})\,. \tag{2.1}$$

Here

$$\underline{K}(\underline{\vec{p}})\equiv\sum_{\alpha=1}^{N}(\underline{\vec{p}}_\alpha)^2/2m\,,$$
$$V(\vec{r})\equiv V(\vec{r}_1,\ldots,\vec{r}_N)\,. \tag{2.2}$$

Here $\underline{K}$ represents the kinetic energy and V represents the potential energy. We consider the case where V is a symmetric function of the position operators $\vec{r}=(\vec{r}_1,\ldots,\vec{r}_N)$. This is not at all required for our purpose, but is assumed for simplicity.

For use later, we also define the plane-wave momentum eigenstates by

$$|\vec{p}\rangle\equiv\psi_{\vec{p}}^{\pm}(\vec{r})$$
$$\equiv\frac{1}{(N!)^{1/2}(2\pi\hbar)^{3N/2}}\sum_P(\pm)^P\prod_{j=1}^{N}\exp(i\vec{p}\cdot\vec{r}_{pj}/\hbar)\,. \tag{2.3}$$

The notation used here is self-explanatory. The eigenvalue $\vec{p}$ should not be confused with the operator $\underline{\vec{p}}$[1].

It will be shown later that it is sufficient to evaluate the matrix element

$$\langle\vec{p}'|\exp(s\underline{H})|\vec{p}\rangle\equiv T(s,\vec{p}',\vec{p})\,. \tag{2.4}$$

It is easily seen that if we let

$$s=-it/\hbar \tag{2.5}$$

we get the transition matrix elements. Also, if we let

$$s=-\beta\,,\qquad |\vec{p}'\rangle=|\vec{p}\rangle\,, \tag{2.6}$$

and sum over the complete set of eigenstates $|\vec{p}\rangle$, we shall get the canonical partition function Z_N,

$$Z_N=\mathrm{Tr}(e^{-\beta\underline{H}})$$
$$=\int(d^3p)T(-\beta,\vec{p},\vec{p})\,. \tag{2.7}$$

Here d^3p stands for

$$\int d^3p\equiv\int\prod_{\alpha=1}^{N}d^3p_\alpha\,.$$

Define now the operator $\underline{U}(s)$ by

$$\underline{U}(s)\equiv\exp(-s\underline{K})\exp(s\underline{H}) \tag{2.8}$$

so that

$$\exp(s\underline{H})=\exp(s\underline{K})\underline{U}(s)\,. \tag{2.9}$$

Substituting (2.9) in (2.4) we get

$$T(s,\vec{p}',\vec{p})=\langle\vec{p}'|e^{s\underline{K}}\underline{U}(s)|\vec{p}\rangle$$
$$=e^{sK(\vec{p}')}\langle\vec{p}'|U(s)|\vec{p}\rangle\,. \tag{2.10}$$

Here $K(\vec{p}')$ is the kinetic energy for momentum $\vec{p}'$, i.e.,

$$K(\vec{p}')=\sum_{\alpha=1}^{N}(\vec{p}'_\alpha)^2/2m\,. \tag{2.11}$$

It follows from Eq. (2.10) that it is sufficient to evaluate

$$\langle \vec{p}' | \underline{U}(s) | \vec{p} \rangle . \tag{2.12}$$

We shall give a very simple method for evaluating this matrix element.

First of all we notice that $\underline{U}(s)$ is a function of the operators $\vec{r}$ and $\vec{p}$ which we write in such a way that any operator $\vec{p}$ is commuted through to the extreme right. Thus there is no position operator $\vec{r}$ to the right of any momentum operator. This can always be done by using the commutation relations. Let the function $U(s)$ when written in such a form be denoted by $\overline{U}(s)$ where

$$\underline{\overline{U}}(s) \equiv \overline{U}(s, \vec{r}, \vec{p}) \equiv \underline{U}(s) . \tag{2.13}$$

The operator $\underline{\overline{U}}(s)$ is exactly equal to the operator $\underline{U}(s)$. However, it is a different function of the operators $\vec{r}$ and $\vec{p}$. This process of rearranging the $\vec{r}$ and $\vec{p}$ operators will always be denoted by a bar over the operator. It follows, therefore, that

$$\begin{aligned} \underline{\overline{U}}(s) | \vec{p} \rangle &= \underline{\overline{U}}(s, \vec{r}, \vec{p}) | \vec{p} \rangle \\ &= \overline{U}(s, \vec{r}, \vec{p}) | \vec{p} \rangle . \end{aligned} \tag{2.14}$$

Here

$$\overline{U}(s) \equiv U(s, \vec{r}, \vec{p})$$

is a classical c-number function of the variables $\vec{r}$ and the eigenvalues $\vec{p}$. It is obtained from the operator $\underline{\overline{U}}(s, \vec{r}, \vec{p})$ by substituting the eigenvalues $\vec{p}$ for the operator $\vec{p}$. Hence,

$$\begin{aligned} T(s, \vec{p}', \vec{p}) = \int d^3 r \exp[sK(\vec{p}')] \overline{U}(s, \vec{r}, \vec{p}) \\ \times \psi^*_{\vec{p}'}(\vec{r}) \psi_{\vec{p}}(\vec{r}) . \end{aligned} \tag{2.15}$$

In (2.15), we have again suppressed the particle index α, so that

$$\int d^3 r \equiv \int \prod_{\alpha=1}^{N} d^3 r_\alpha .$$

Let us now define a function $\overline{V}$ such that

$$\overline{U}(s, \vec{r}, \vec{p}) \equiv \exp\{s[\overline{V}(s, \vec{r}, \vec{p}) + V(\vec{r})]\} . \tag{2.16}$$

Such a function $\overline{V}$ may always be defined if we know $\overline{U}$; note that $V(\vec{r})$ is the potential defined in (2.2). It follows from (2.15) and (2.16) that

$$\begin{aligned} T(s, \vec{p}', \vec{p}) = \int d^3 r \exp[sE(\vec{p}', \vec{r}) + s\overline{V}(s, \vec{r}, \vec{p})] \\ \times \psi^*_{\vec{p}'}(\vec{r}) \psi_{\vec{p}}(\vec{r}) . \end{aligned} \tag{2.17}$$

Here E is the c-number function which is exactly equal to the classical energy, i.e.,

$$E(\vec{p}', \vec{r}) \equiv \sum_{\alpha=1}^{N} (\vec{p}'_\alpha)^2 / 2m + V(\vec{r}_1, \ldots, \vec{r}_N) . \tag{2.18}$$

The c-number function $\overline{V}$ is a correction to the classical energy E. The function $\overline{V}$ approaches zero in the correspondence limit ($\hbar \to 0$).

In (2.17) we have resolved the problem of evaluating the matrix element to that of a $3N$-dimensional integral over the configurational space. In general, $\overline{V}$ may not be evaluated exactly. The customary perturbation series amounts to an expansion of $\overline{U}$ in powers of the coupling constant. We instead develop a method in which the function $\overline{V}$ is expanded in powers of the coupling constant. This evidently leads to an entirely new method of self-consistent approximations. In general, the expansion for $\overline{V}$ need not converge rapidly. However, for most cases of physical interest this series converges much more rapidly than the customary series for $\overline{U}$. This point is discussed in detail in Sec. IV.

III. THE EFFECTIVE HAMILTONIAN

In the previous section we had resolved the problem of evaluating the matrix element $T(s, \vec{p}', \vec{p})$ to that of a simple classical integral. To make use of this equation we must find $\overline{V}$, which is a c-number function, in terms of the potential V. For this purpose we start with the definition (2.8), viz.,

$$\underline{U}(s) = \exp(-s\underline{K}) \exp(s\underline{H}) . \tag{2.8}$$

Differentiate (2.8) with respect to s. We get

$$\frac{d\underline{U}(s)}{ds} = \underline{H}_1(s) \underline{U}(s) , \tag{2.8'}$$

where

$$\underline{H}_1(s) \equiv \exp(-s\underline{K}) V \exp(s\underline{K}) . \tag{3.1}$$

Integrating (2.8′) with respect to s we get

$$\underline{U}(s) = 1 + \int_0^s ds_1 \underline{H}_1(s_1) \underline{U}(s_1) . \tag{3.2}$$

Here, we have used the boundary condition that

$$\underline{U}(s) = 1 \quad \text{when } s = 0 . \tag{3.3}$$

It is not possible to solve exactly the integral equation (3.2). It can be written as

$$\begin{aligned} \underline{U}(s) &= \sum_{n=0}^{\infty} \int_0^s ds_1 \cdots \int_0^{s_{n-1}} ds_n \underline{H}_1(s_1) \cdots \underline{H}_1(s_n) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^s ds_1 \cdots \int_0^s ds_n \mathcal{S}(\underline{H}_1(s_1) \cdots \underline{H}_1(s_n)) . \end{aligned} \tag{3.4}$$

Here we define the s-ordering operator $\mathcal{S}$ in exactly the same form as the time-ordering operator T in field

theory.

From the definition of $\bar{U}(s, \vec{r}, \vec{p})$ it follows that

$$U(s, \vec{r}, \vec{p}) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^s ds_1 \int_0^s | ds_n \mathcal{S}[H_1(s_1) H_1(s_n)]_{\text{comm}}$$

where

$$\bar{H}_n(s_1, s_n) \equiv H_n \equiv [H_1(s_1) \cdots H_1(s_n)]_{\text{comm}}. \tag{3.5}$$

In this expression $[\ ]_{\text{comm}}$ denotes the fact that we have to commute all the momentum operators to the extreme right and replace the operator $\vec{p}$ by its eigenvalue $\vec{p}$. It is thus sufficient to evaluate $\bar{H}_n$ defined in (3.5).

The details for evaluating $\bar{H}_n$ are given in the Appendix. It is shown that

$$H_n = \int_0^s ds_1 \cdots \int_0^s ds_n \mathcal{S} \left\{ \prod_{j=1}^{n} \left[V\left(\vec{r}_j - \frac{s_j \hbar}{mi} \vec{p}\right) \exp\left(-\frac{s_j \hbar^2}{2m} \vec{D}_j^{\,2}\right) \prod_{l=j+1}^{n} \exp\left(\frac{-s_j \hbar^2}{m} \vec{D}_j \cdot \vec{D}_l\right) \right] \right\}. \tag{3.6}$$

Here $\vec{r}_j$ is to be set equal to $\vec{r}$ after operating with $\vec{D}_j$, which is defined by

$$\vec{D}_j f(\vec{r}_k) \equiv \delta_{jk} \frac{\partial f(\vec{r})}{\partial \vec{r}}. \tag{3.7}$$

In (3.7) the index j should not be confused with the particle index α, defined in (2.2). Here j is a dummy index. The formula with the particle index put back is given in Sec. 1 of the Appendix.

Define now

$$K_{jl}(s_j) \equiv -1 + \exp\left(-\frac{s_j \hbar^2}{m} \vec{D}_j \cdot \vec{D}_l\right), \quad j < l \tag{3.8}$$

and let

$$V_0(j) \equiv V\left(\vec{r}_j - \frac{s_j \hbar \vec{p}}{mi}\right) \exp\left(-\frac{s_j \hbar^2}{2m} \vec{D}_j^{\,2}\right). \tag{3.9}$$

It follows from (3.7), (3.8), and (3.9) that

$$\begin{aligned} \bar{U}(s) &= \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^s ds_1 \cdots \int_0^s ds_n \prod_{j=1}^{n} V_0(j) \mathcal{S} \left[\prod_{j=1}^{n} \prod_{l>j}^{n} [1 + K_{jl}(s_j)] \right] \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^s ds_1 \cdots \int_0^s ds_n \prod_{j=1}^{n} V_0(j) \mathcal{S} \left[\prod_{j=1}^{n} \prod_{l>j}^{n} [1 + K_{jl}(s_j)] \right]. \end{aligned} \tag{3.10}$$

The series (3.10) for $\bar{U}(s)$ can be easily summed up by using the linked-cluster method of summation introduced by Mayer.[2] We now introduce the necessary terminology and the method for calculating the linked-cluster terms. These are functions of $\vec{r}$, $\vec{p}$ and s.

A linked-cluster diagram of order l is drawn in the following way:

(i) Draw l points and number them from -1 to l. This is best done by choosing the end-points of a polygon of degree l. These points are called the vertices.

(ii) Connect the vertices by lines, each line joining two points, with a direction from the lower-numbered point to the higher-numbered point. These lines are called the propagators.

(iii) A diagram is called irreducible if we may reach an arbitrary point Q starting from an arbitrary point P, simply by following along the lines drawn in (ii). We need not follow a line along its direction.

This gives us the method of drawing the diagrams. In order to calculate the value of each diagram we have the following rules.

(i) For each vertex j write a factor $V_0(j)$ defined in Eq. (3.10).

(ii) For a propagator joining the vertices j and l, with $j < l$, i.e., in the direction j to l apply the operator $K_{jl}(s_j)$, between the vertices j and l.

(iii) Apply the $\mathcal{S}$ ordering operator, defined in Eq. (3.5), on the propagators $K_{jl}(s_j)$.

(iv) The expression obtained in (i), (ii), and (iii) is then integrated over the variables s_1, $s_2, \ldots, s_n$ each between the limits 0 and s.

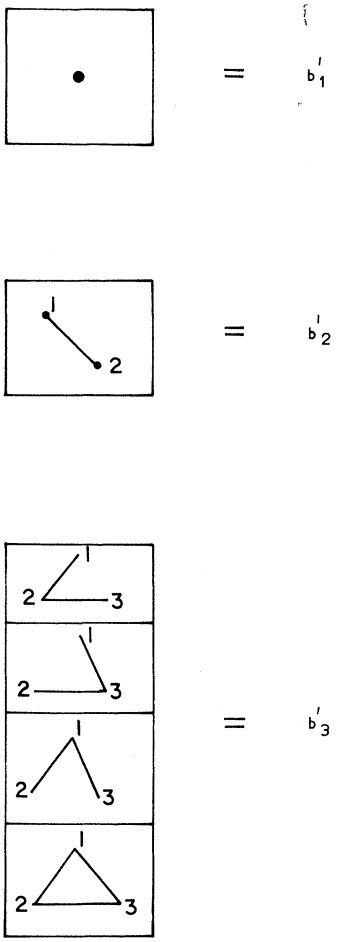

FIG. 1. The linked-cluster diagrams.

The result obtained above is called the linked-cluster value $F^{(G)}$ of the diagram G. The sum $F^{(G)}$ over all irreducible diagrams, G of order l, and divided by $l!$, is called the value of the linked-cluster function, b_l, of order l. That is,

$$b_l \equiv b_l(s, \vec{r}, \vec{p}) = \frac{1}{l!} \sum_G F^{(G)} . \tag{3.11}$$

The irreducible diagrams for b_1, b_2 and b_3 are drawn in Fig. 1.

It immediately follows for the Mayer's method of summation that

$$\overline{U}(s) = \exp\left[\sum_{l=1}^{\infty} b_l(s, \vec{r}, \vec{p})\right] . \tag{3.12}$$

Hence, from (2.16)

$$\overline{V}(s, \vec{r}, \vec{p}) = \frac{1}{s} \sum_{l=1}^{\infty} b_l(s, \vec{r}, \vec{p}) - V(\vec{r}) . \tag{3.13}$$

If we substitute the value of $\overline{V}$ obtained in (3.14) into Eq. (2.15), we get

$$T(s) \equiv T(s, \vec{p}', \vec{p}) = \int d^3r \exp[s(E(\vec{p}', \vec{r}) + V(s, \vec{r}, \vec{p}))] \psi^*_{\vec{p}'}(\vec{r}) \psi_{\vec{p}}(\vec{r}) . \tag{3.14}$$

This expression for $T(s)$ has very interesting properties which are discussed in the next section.

IV. DISCUSSION

A simple expression is given for the matrix element in Sec. III, Eq. (3.15). The expression for $\overline{V}$ is an infinite series. In general, it is not possible to find a closed-form expression for $\overline{V}$. We shall assume that the series for $\overline{V}$ is convergent and possesses all the nice mathematical properties required of it. We now make some interesting observations.

(a) The linked-cluster function b_l is dimensionless.

(b) The function b_l is proportional to the lth power of the coupling constant. This is so for a diagram for b_l has at least l vertices and there is a factor V_0 at each of these vertices.

(c) A self-consistent method of approximation is obtained if we keep the first few terms in the series (3.14) for $\overline{V}$.[3,4]

(d) It follows from the definition (3.9) that K_{jl} is a power series in $\hbar$, with the first term proportional to $\hbar$. Hence it vanishes as $\hbar \to 0$.

(e) Since an irreducible diagram of order l has at least $(l-1)$ propagators K_{jl}, it follows that b_l vanishes as $(\hbar)^{l-1}$ when $\hbar \to 0$.

(f) Since $\hbar$ is small, it may be sufficient to keep terms only up to a given power of $\hbar$. This will be a good approximation if the potential $V(\vec{r})$ is a slowly varying function. This is so, because each power of $\hbar$ is associated with one simple derivative of $V(\vec{r})$, which comes from K_{jl}.

(g) The method of self-consistent field approximation developed for the many-body systems[3,4] and for the anharmonic crystal[3,4] may be quite profitably applied to find various partial sums of the series (3.14).

This will be shown in detail in later papers.

Consider now Eq. (2.7) which defines the canonical partition function Z_N. It may be written as

$$Z_N = \int d^3p d^3r \exp\{-\beta[E(\vec{p}, \vec{r}) + \overline{V}(-\beta, \vec{r}, \vec{p})]\} S(\vec{p}, \vec{r}) . \tag{4.1}$$

Here,

$$S(\vec{p}, \vec{r}) \equiv |\psi_{\vec{p}}(\vec{r})|^2 . \tag{4.2}$$

The function V is a symmetric function of its arguments, since the system contains N identical particles. It follows that it is independent of the

statistics. Further note that $\overline{V} \to 0$ as $\hbar \to 0$, i.e., in the limit when position and momentum operators commute. Hence, $\overline{V}$ (Ref. 5) gives all the corrections to the classical energy function $E(\vec{p}, \vec{r})$, which are due to the noncommutativity of the position and momentum operators. These we call quantum corrections.

If we look at the definition (4.2) of the $S(\vec{p}, \vec{r})$ we note that it is a positive definite function of its arguments. If we assume Maxwell-Boltzmann statistics, we find that

$$S(\vec{p}, \vec{r}) = 1/[(N!(2\pi\hbar)^{3N}]. \tag{4.3}$$

In the case of Fermi-Dirac and Bose-Einstein statistics we similarly get different functions of $\vec{p}$ and $\vec{r}$. Note that $S(p, r)$ depends on $\hbar$. The corrections due to using Fermi-Dirac and Bose-Einstein statistics instead of the Maxwell-Boltzmann statistics depend on powers of $\hbar$. Such corrections will be called statistical corrections.

We recall that $\overline{V}$ is independent of statistics. Since there is an integral over phase space in Eq. (4.1) it follows that Z_N will contain products of the quantum and statistical corrections. However, these can be taken care of by writing h' for Planck's constant in $S(\vec{p}, \vec{r})$.

In certain calculations it may be sufficient to neglect all the quantum corrections and keep to statistical corrections exactly. Such situations arise at low temperatures. On the other hand at high temperatures, statistics is not very important, and, hence, we may use the Maxwell-Boltzmann statistics with the quantum corrections taken completely. Note that at high temperatures β is very small. The integrals for b_l may be easily done by expansion in powers of the integrating variable $s_j = -\beta_j$.

Let us study Eq. (4.11), which gives the canonical partition function Z_N in quantum statistical mechanics. It is easily seen that the result may be interpreted as a classical canonical partition function with

(i) a positive definite density $S(\vec{p}, \vec{r})$, and

(ii) an effective Hamiltonian

$$H_{\text{eff}}(-\beta, \vec{r}, \vec{p}).$$

The effective Hamiltonian depends on the temperature. Nevertheless, we may make an interesting observation:

Quantum statistical mechanics is equivalent to classical statistical mechanics.

This is a very surprising result. We shall not comment on it any further. Whether a similar conclusion holds for the nonrelativistic quantum mechanics is a debatable point. Keeping in mind the well-known von Neumann's theorem, such a conclusion need not be valid. A full discussion of this point is outside the scope of this paper, and is left for future investigation.

V. CONCLUSION

Starting with a spin-independent Hamiltonian H, we calculated the matrix element of $\exp(+sH)$; here s is a c-number parameter. The problem was reduced to that of calculating a phase-space integral, the integrand being the product of $\exp(+sH_{\text{eff}})$ with $\psi^*_{\vec{p}'}(r)\psi_{\vec{p}}(\vec{r})$. We therefore need to calculate H_{eff}, which is a c-number function of s, $\vec{r}$, and $\vec{p}$. In general, H_{eff} cannot be calculated exactly. However, we have suggested a method for doing self-consistent approximations. Arguments for this are given in Sec. IV. A diagrammatic approach is also given in this section.

The formalism is easily applied to the calculation of the transition amplitude and the quantum partition function. The method for calculating the matrix elements of an arbitrary operator is given in the Appendix.

It is evident from (4.1) that quantum statistical mechanics is equivalent to an equivalent problem in classical statistical mechanics; we admit temperature-dependent classical Hamiltonians.

There are no general methods for numerically calculating the integrals occurring in $T(s)$, Eq. (3.15). It is easily seen that integral over d^3r amounts to taking a Fourier transform of $\exp(+sH_{\text{eff}})$. The d^3p integral may similarly be interpreted as the volume of the Fourier transform in the momentum space.

Lastly we remark that spin may also be included in the above formalism. Further, an extension to the many-body theory and the relativistic quantum field theory is possible. This will form the subject matter of the next paper in this series. We hope to be able to calculate a large number of physical variables by this method.

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APPENDIX: DETAILS OF THE CALCULATIONS

1. Evaluation of H_n

We give a method for calculating the function H_n defined in Eq. (3.5). From Eq. (3.1),

$$\underline{H}_1(s) = \exp(-s\underline{K})V\exp(s\underline{K}).$$

Now

$$\exp(-s\underline{K})\vec{\mathrm{r}}\exp(s\underline{K}) = \vec{\mathrm{r}} - \frac{s\hbar}{mi}\vec{\mathrm{p}}\,. \tag{A1}$$

This gives us

$$\begin{aligned}\underline{H}_1(s) &= V\left(\vec{\mathrm{r}} - \frac{s\hbar}{mi}\vec{\mathrm{p}}\right)\\ &= \sum_{n=0}^{\infty}\frac{1}{2^n}\sum_{j=0}^{n}\frac{1}{j!}\frac{1}{(n-j)!}\left(-\frac{s\hbar}{mi}\vec{\mathrm{p}}\right)^{j}\\ &\quad\times\frac{\partial^n V}{\partial r^n}\left(-\frac{s\hbar}{mi}\vec{\mathrm{p}}_m\right)^{n-j}\\ &= \exp\left(-\frac{s\hbar}{2mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}\right)V(\vec{\mathrm{r}})\exp\left(-\frac{s\hbar}{2mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}\right).\end{aligned} \tag{A2}$$

This is changed by changing the order of the n and j summations and then letting $n \to n+j$. The operator $\vec{\mathrm{D}}$ occurring in (A2) is defined by

$$\vec{\mathrm{D}}f(\vec{\mathrm{r}}) \equiv \frac{\partial f(\vec{\mathrm{r}})}{\partial \vec{\mathrm{r}}}\,. \tag{A3}$$

From (A2) it follows that

$$\begin{aligned}\underline{H}_1(s) &= \exp\left(-\frac{s\hbar}{2mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}\right)V(\vec{\mathrm{r}})\exp\left(-\frac{s\hbar}{2mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}\right)\\ &= \exp\left(-\frac{s\hbar}{2mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}\right)V(\vec{\mathrm{r}})\exp\left(\frac{s\hbar}{2mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}\right)\\ &\quad\times\exp\left(-\frac{s\hbar}{mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}\right).\end{aligned} \tag{A4}$$

In (A4) we have used the identity

$$\exp(-\vec{\mathrm{a}}\cdot\vec{\mathrm{p}})V(\vec{\mathrm{r}})\exp(\vec{\mathrm{a}}\cdot\vec{\mathrm{p}}) = V(\vec{\mathrm{r}})\exp\left(+\frac{\hbar}{i}\vec{\mathrm{a}}\cdot\vec{\mathrm{D}}\right). \tag{A5}$$

Here $\vec{\mathrm{a}}$ is an operator which commutes with $\vec{\mathrm{p}}$.

The function H_n is easily obtained from (A4). By definition (3.5),

$$\begin{aligned}H_n &= [H_1(s_1)\cdots H_1(s_n)]_{\text{comm}}\\ &= \prod_{j=1}^{n} V(r_j)\exp\left(\frac{s_j\hbar^2}{2m}\vec{\mathrm{D}}_j^{\,2}\right)\exp\left(-\frac{s_j\hbar}{mi}\vec{\mathrm{p}}\cdot\vec{\mathrm{D}}_j\right)\\ &\quad\times\prod_{l>j}^{n}\exp\left(-\frac{s_j\hbar}{m}\vec{\mathrm{D}}_j\vec{\mathrm{D}}_l\right).\end{aligned} \tag{A6}$$

Here we have used (A5). Note that after applying the operator $\vec{\mathrm{D}}_j$ replace $\vec{\mathrm{r}}_j$ by $\vec{\mathrm{r}}$, the actual coordinates; j is just a dummy index.

Putting back the particle index in (A6), we replace

$$\exp\left(-\frac{s\hbar^2}{m}\vec{\mathrm{D}}_j^{\,2}\right) \equiv \prod_{\alpha=1}^{N}\exp\left(-\frac{s\hbar^2}{m}(\vec{\mathrm{D}}_{j\alpha})^2\right),$$

$$\exp\left(-\frac{s\hbar^2}{m}\vec{\mathrm{D}}_j\vec{\mathrm{D}}_l\right) = \prod_{\alpha=1}\exp\left(-\frac{s\hbar^2}{m}\vec{\mathrm{D}}_{j\alpha}\cdot\vec{\mathrm{D}}_{l\alpha}\right),$$

$$V(\vec{\mathrm{r}}_j) = V(\vec{\mathrm{r}}_{j1}, \vec{\mathrm{r}}_{j2}, \ldots, \vec{\mathrm{r}}_{j\alpha}, \ldots, \vec{\mathrm{r}}_{jN})\,.$$

Let us now consider $V_0(j)$ defined in Eq. (3.9). Taking the Fourier transform we get

$$\begin{aligned}V_0(r) &= \int\frac{d^3k}{(2\pi)^{3/2}}V(\vec{\mathrm{k}})\\ &\quad\times\exp\left[-i\vec{\mathrm{k}}\left(\vec{\mathrm{r}} - \frac{s\hbar}{mi}\vec{\mathrm{p}}\right) + \frac{s\hbar^2}{2m}k^2\right].\end{aligned} \tag{A7}$$

Here $V(\vec{\mathrm{k}})$ is the Fourier transform of $V(\vec{\mathrm{r}})$. We have suppressed the particle index in the above formula. This integral will always exist provided the integral

$$\left|\int d^3k\, V(\vec{\mathrm{k}})\exp\left(\frac{s\hbar\vec{\mathrm{k}}\vec{\mathrm{p}}}{m} + \frac{s\hbar^2\vec{\mathrm{k}}^2}{2m}\right)\exp(-i\vec{\mathrm{k}}\vec{\mathrm{r}})\right| < \infty \tag{A8}$$

uniformly in s. Note that s is either positive or purely imaginary. The integral (A7) exists for all potentials of physical importance. Hence $V_0(r)$ is well defined.

2. Solution to the Schrödinger Equation

The method we have developed in the text can be easily used to find a solution to the Schrödinger equation. In particular, if we know $\overline{V}(s, \vec{\mathrm{r}}, \vec{\mathrm{p}})$ we may write the solution in the form

$$\begin{aligned}\psi(\vec{\mathrm{r}}, t) = \int d^3p\Bigg\{&\exp\left[-\frac{it}{\hbar}\left(\frac{p^2}{2m} + \overline{V}\left(-\frac{it}{\hbar}, \vec{\mathrm{r}}, \vec{\mathrm{p}}\right)\right)\right]\\ &\times\exp\left(-\frac{i\vec{\mathrm{p}}\cdot\vec{\mathrm{r}}}{\hbar}\right)\psi_0(\vec{\mathrm{p}})\Bigg\}.\end{aligned} \tag{A9}$$

Here $\psi_0(\vec{\mathrm{p}})$ is the initial state of the system at time $t=0$, in the momentum representation. Further $\psi(\vec{\mathrm{r}}, t)$ is the solution in the coordinate representation at the time t. Thus the solution is obtained by a simple quadrature over the momentum variables if $\overline{V}$ is known.

We may give the function $\overline{V}$, instead of the potential V, as our input function. This will lead to a simple solution to the scattering problem for the nonrelativistic spin-zero Hamiltonian.

3. Matrix Element of an Operator

We shall now find the matrix element of an arbitrary operator $\underline{F}(\vec{\mathrm{r}}, \vec{\mathrm{p}})$. Let us calculate the matrix element between two momentum wave functions $\psi_{\vec{\mathrm{p}}'}(\vec{\mathrm{r}})$ and $\psi_{\vec{\mathrm{p}}}(\vec{\mathrm{r}})$, which are defined in (2.3). The matrix element $F(\vec{\mathrm{p}}', \vec{\mathrm{p}})$ is given by

$$F(\vec{\mathrm{p}}', \vec{\mathrm{p}}) = \int d^3r\,\psi_{\vec{\mathrm{p}}'}(r)\overline{F}(\vec{\mathrm{r}}, \vec{\mathrm{p}})\psi_{\vec{\mathrm{p}}}(\vec{\mathrm{r}})\,. \tag{A10}$$

Let us now define $\overline{F}$ in a way similar to $\overline{U}$ in the text:

$$\underline{\overline{F}}(\vec{\mathrm{r}}, \vec{\mathrm{p}})\psi_{\vec{\mathrm{p}}}(\vec{\mathrm{r}}) = \overline{F}(\vec{\mathrm{r}}, \vec{\mathrm{p}})\psi_{\vec{\mathrm{p}}}(\vec{\mathrm{r}})\,. \tag{A11}$$

Substituting (A11) in (A10) we get

$$\overline{F}(\vec{p}', \vec{p}) = \int d^3r \, \psi_{\vec{p}'}(\vec{r}) \psi_{\vec{p}}(r) \overline{F}(\vec{r}, \vec{p}) .$$

This amounts to taking a simple Fourier transformation of $\overline{F}(\vec{r}, \vec{p})$ which is a c-number function.

4. Particular Cases

We shall consider two particular examples of the potential $V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$; these occur very often in quantum statistical mechanics. The two cases are

(I) one-body potential,
(II) two-body potential.

The cases when the potential V is a sum of potentials of the form (I) and (II) may also be treated similarly. We give a new set of diagrams which may be easily generalized to an arbitrary l-body potential ($1 \leq l \leq N$). First, let us consider (I) and (II).

Case (I). One-Body Potential

Let

$$V(\vec{r}) = \sum_{\alpha=1}^{N} V^{(1)}(\vec{r}_\alpha) .$$

Here $V^{(1)}$ is a one-body potential. The total Hamiltonian $H^{(N)}$ (denoted simply by H in the text) is given by

$$\underline{H}^{(N)} = \sum_{\alpha=1}^{N} [\underline{\vec{p}}_\alpha^{\,2}/2m + V^{(1)}(\vec{r}_\alpha)] . \tag{A12}$$

Here N refers to the number of particles. The Hamiltonian $H^{(N)}$ is the sum of N single-particle Hamiltonians $H^{(1)}$ where

$$\underline{H}^{(1)}(\underline{\vec{p}}_\alpha, \vec{r}_\alpha) = \underline{\vec{p}}_\alpha^{\,2}/2m + V^{(1)}(\vec{r}_\alpha) . \tag{A13}$$

In order to calculate $H_{\text{eff}}^{(N)}$, it is sufficient to calculate $H_{\text{eff}}^{(1)}$, for

$$H_{\text{eff}}^{(N)} = \sum_{\alpha=1}^{N} H_{\text{eff}}^{(1)}(s, \vec{p}_\alpha, \vec{r}_\alpha) . \tag{A14}$$

This is so since the commutator

$$[H^{(1)}(\vec{p}_\alpha, \vec{r}_\alpha), H^{(1)}(\vec{p}_\beta, \vec{r}_\beta)] = 0 . \tag{A15}$$

The function $H_{\text{eff}}^{(1)}$ may be easily obtained by considering the diagrams (Fig. 1). We, of course, draw these diagrams for the single-particle Hamiltonian $H^{(1)}$. The graphs rule are same, and now

$$V_0(j) = V^{(1)}\left(\vec{r}_j - \frac{s_j \hbar \vec{p}}{mi}\right) \exp(-s_j \hbar^2 / 2m \vec{D}_j^{\,2}) . \tag{A16}$$

Here j is a dummy index and should not be confused with the particle index.

It immediately follows from the above discussion that

$$b_l(\vec{r}_\alpha, \vec{p}_\alpha) = \sum_{\alpha=1}^{N} b_l^{(1)}(\vec{r}_\alpha, \vec{p}_\alpha) . \tag{A17}$$

Here $b_l^{(1)}$ is the linked-cluster expression for the l-order diagram for the Hamiltonian $\underline{H}^{(1)}(\underline{\vec{p}}, \vec{r})$ of a single particle.

The task of calculating the linked-cluster sum for one-body potentials thus becomes very simple.

Case (II). Two-Body Potential

Let now

$$V = \sum_{\alpha<\beta}^{N} V^{(2)}(\vec{r}_\alpha, \vec{r}_\beta) .$$

The function $V_0(j)$ is now

$$V_0(j) = \sum_{\alpha<\beta} V^{(2)}(\vec{r}_{j\alpha} - s_j \hbar \vec{p}_\alpha / mi, \vec{r}_{j\beta} - s_{j\alpha} \hbar \vec{p}_\beta / mi) \exp\left(-s_j \frac{\hbar^2}{2m} \vec{D}_j \cdot \vec{D}_j\right)$$

$$= \sum_{\alpha<\beta} V_0^{(2)}(j; \alpha, \beta; s_j) , \tag{A18}$$

where

$$V_0^{(2)}(j; \alpha, \beta; s_j) \equiv V_0^{(2)}(\vec{r}_{j\alpha} - s_j \hbar \vec{p}_\alpha / mi; \vec{r}_{j\beta} - s_j \hbar \vec{p}_\beta / mi) \exp[(-s_j \hbar^2 / 2m)(\vec{D}_{j\alpha} \cdot \vec{D}_{j\alpha} + \vec{D}_{j\beta} \cdot \vec{D}_{j\beta})] . \tag{A19}$$

We now give explicit forms for b_1 and b_2, and then a method for evaluating b_n, showing that it is a sum of l-body potentials with $l \leq 2n - 1$.

From the text it follows that

$$b_1 = \frac{1}{1!} \int_0^s ds \sum_{\alpha<\beta} V_0^{(2)}(j; \alpha, \beta; s_1)$$

$$= \sum_{\alpha<\beta} b_1^{(2)}(\alpha, \beta) . \tag{A20}$$

Here

$$b_1^{(2)}(\alpha,\beta)=\frac{1}{1!}\int_0^s ds_1 V_0^{(2)}(j;\alpha,\beta;s_1)\,. \tag{A21}$$

It is obviously a two-body potential.

Next we have from Eq. (3.11) that

$$b_2=\frac{1}{2!}\int_0^s ds_1\int_0^{s_1} ds\, V_0(1)V_0(2)K_{12}(s_1)\,. \tag{A22}$$

From Eq. (A19),

$$\begin{aligned}V_0(1)V_0(2)K_{12}(s_1) &= \sum_{\alpha_1<\beta_1;\,\alpha_2<\beta_2} V_0^{(2)}(1;\alpha_1,\beta_1;s_1)V_0^{(2)}(2;\alpha_2,\beta_2;s_2)\{\exp[(-\hbar^2/2m)\textstyle\sum_\alpha s_1\vec{D}_{1\alpha}\cdot\vec{D}_{2\alpha}]-1\}\\ &= \sum_{\alpha<\beta_1,\beta_2;\,\beta_1\neq\beta_2} V_0^{(2)}(1;\alpha,\beta_1;s_1)V_0^{(2)}(2;\alpha,\beta_2;s_2)K_{12}^{(\alpha)}(s_1)K_{12}^{(\beta_1)}(s_1)K_{12}^{(\beta_2)}(s_1)\\ &\quad+\sum_{\alpha_1,\alpha_2<\beta;\,\alpha_1\neq\alpha_2} V_0^{(2)}(1;\alpha_1,\beta;s_1)V_0^{(2)}(2;\alpha_2,\beta;s_2)K_{12}^{(\alpha_1)}(s_1)K_{12}^{(\alpha_2)}(s_1)K_{12}^{(\beta)}(s_1)\\ &\quad+\sum_{\alpha<\beta} V_0^{(2)}(1;\alpha,\beta;s_1)V_0^{(2)}(2;\alpha,\beta;s_2)K_{12}^{(\alpha)}(s_1)K_{12}^{(\alpha)}(s_1)K_{12}^{(\beta)}(s_1)\,.\end{aligned} \tag{A23}$$

The notation is explained in Eq. (A18). Thus,

$$b_2=\frac{1}{2!}\sum_{\alpha<\beta<\gamma} b_2^{(3)}(\alpha,\beta,\gamma)+\frac{1}{2!}\sum_{\alpha<\beta} b_2^{(2)}(\alpha,\beta)\,. \tag{A24}$$

Here $b_2^{(3)}$ is the sum of the first two terms and clearly depends on these coordinates, i.e., that it is a three-body potential; the suffix (3) on $b_2^{(3)}$ denotes that it is a three-body potential, while the subscript 2 denotes that it contributes to the link-cluster term of order two. Similarly, $b_2^{(2)}$ denotes a two-body potential. Also,

$$K_{jl}^{(\alpha)}(s_j)=\exp[(-s_j\hbar^2/m)(D_j^{(\alpha)}\cdot D_l^{(\alpha)})]-1\,. \tag{A25}$$

In Eq. (A24), the s integrations are assumed to be done. Further, we have supposed dependence on the s variables. From now on we shall completely suppress dependence on the s variables.

We shall now derive a similar result for an arbitrary linked-cluster function b_n. Draw the following diagram (Fig. 2).

(i) There are N points in each horizontal row, corresponding to N particles.

(ii) There are n such horizontal rows corresponding to order n of the linked-cluster expansion.

(iii) Draw all linked-cluster diagrams of order n, as is explained in the text. Let these be k in number and denote them by $G^{(n)}(1)$, $G^{(n)}(2),\ldots,$ $G^{(n)}(k)$. Each diagram $G^{(n)}(m)$ has the operators $K_{j_1l_1},\ldots,K_{j_ml_m}$ acting on it.

(iv) A typical diagram $G^{(n)}(m)$ gives us

$$V_0(j)K_{j_1l_1}(s_{j_1})\cdots K_{j_ml_m}(s_{j_m})\,. \tag{A26}$$

For a two-body potential a typical term in the product $V_0(j)$ is

$$V_0^{(2)}(\alpha_1,\beta_1)\cdots V_0^{(2)}(\alpha_n,\beta_n)$$

with $\alpha_i<\beta_i$.

(v) In Fig. 2, draw a line connecting the point α_i with β_i in the ith row. We note that

$$V_0^{(2)}(j;\beta,\gamma)K_j^{(\alpha)}(s_j)=0$$

if $\alpha\neq\beta,\quad \alpha\neq\gamma$. (A27)

(vi) It therefore follows that, in order that a term be nonzero, at least two of the n indices α_1, α_2, $\alpha_3,\ldots,\alpha_n$ must be equal, or at least two of the indices β_1, β_2, $\beta_3,\ldots,\beta_n$ must be equal, or they may be jointly equal

We now give the graph rules.

(1) Form the pair of points (α_j,β_j) in the jth column.

(2) In each column connect the points s_1, $s_2,\ldots,$

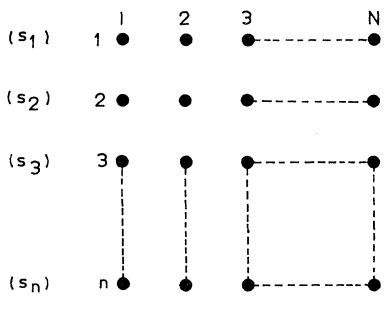

FIG. 2. The particle-number diagrams.

s_n in an arbitrary manner. Some examples are given in Fig. 3. Some of the points remain unconnected and some are connected to more than one point.

(3) For each vertical line connecting the jth and lth row in the column, introduce the operator $K_{jl}^{(\alpha)}(s_j)$ with $j < l$. This acts on $V_0^{(2)}(j; \alpha_j, \beta_j; s_j)$.

(4) Sum up over all possible pairings (α_j, β_j) in each horizontal row (the jth row).

(5) We shall now obtain a many-particle potential $b_n^{(l)}$ with $l \leq 2n-1$. The value of l depends on how many of the points are vertically connected. Thus for b_3, for the first linked-cluster diagram (Fig. 1), we shall have a potential which is such that there are three points which are mutually connected. This gives us a sum of the two, three, four, and five-body potentials.

If $(j+1)$ points are vertically connected, then

$$l = 2n - j .$$

Thus the nth linked-cluster diagrams yield an expression for b_n which is a sum of l-body potentials with $l \leq 2n-1$.

We may similarly treat the case when $V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$ is a sum of l-body potentials. That is

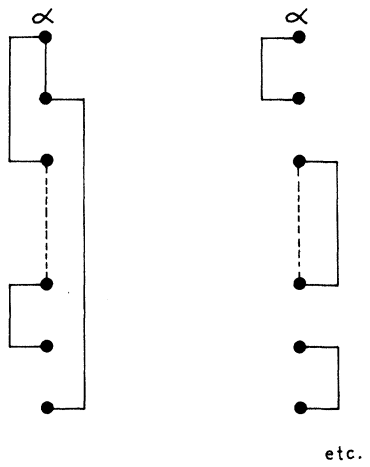

FIG. 3. Particle-number dependence.

$$V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{\alpha_1 < \alpha_2 \cdots < \alpha_l} V^{(l)}(\vec{r}_{\alpha_1}, \vec{r}_{\alpha_2}, \ldots, \vec{r}_{\alpha_l}) .$$

In this case we have to pair points $\alpha_1, \alpha_2, \ldots, \alpha_l$ in each horizontal row and then proceed as in the above case.

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[1]An operator is always underlined. Thus $\underline{\vec{R}}$ represents a vector operator and $\vec{R}$ represents an eigenvalue of the operator $\underline{\vec{R}}$.

[2]K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).

[3]L. Van Hove, MIT lecture notes (unpublished).

[4]P. Choquard, *The Anharmonic Crystal* (Benjamin, New York, 1967). See this for other references.

[5]Anil C. Rae, M. S. Thesis submitted to the University of Minnesota, 1964 (unpublished). The function $\bar{U}$ was first introduced here.