STUDIES IN THE MANY-BODY PROBLEM IN QUANTUM MECHANICS

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SUMMARY

One of the more important aspects of the many-body problem in Quantum Mechanics is that of determining the properties of a Bose system of particles with repulsive interactions. Several investigators have treated this particular problem using newer perturbation methods in the formalism of second quantization. The presence of formal complications when conventional perturbation methods are applied to many-particle systems has led to the development of newer different perturbation methods. More recently, the same problem has been considered dealing directly with the wave function in configuration space, using the theory of cluster expansions first introduced in statistical mechanics. In these latter treatments the ground state wave function is expressed as a product of pair functions. The problem of evaluating the expectation value for the energy then becomes analogous to evaluating the classical partition function for an imperfect gas, expressed in terms of Mayer's cluster integrals. By considering only contributions to the energy from the ring cluster integrals, a tractable expression for the ground state energy at low densities is obtained. Then a choice for the pair function is made and subsequent variation with respect to a parameter in the chosen trial function has been shown to yield a ground state energy quite close to the exact asymptotic expression obtained from perturbation theory in the formalism of second quantization, where the contribution to the ground state energy from pair excitations was calculated exactly.

Now one might naturally ask how this cluster integral method in configuration space is related to the perturbation theory calculation using

momentum-space eigenfunctions. An analogous situation exists for the calculation of the partition function of an ideal Bose gas, where there is a cluster integral development which is completely equivalent to the more usual sum-over-states. One might expect that here as well, the pair approximation perturbation theory should have its exact counterpart in a configuration space cluster integral treatment. The primary purpose of the present investigation is to show that this expectation is indeed fulfilled. The cluster integral calculations previously made are not directly comparable to the perturbation theory calculations simply because the class of ring integrals which were taken as contributing to the ground state energy do not correspond to the pair approximation of perturbation theory. This pair approximation yields a ground state which in configuration space has been shown by Lee, Huang, and Yang to have the form

$$\Phi = \prod_{i<j=1}^{N}{}' \left[1 + f(r_{ij})\right]$$

where the prime denotes that in the expanded product for all terms with repeated particle indices are omitted. The prohibition of repeated particle indices is essential for the pair excitation approximation, since the Fourier transform of a term with one repeated index, such as $f(r_{12})\ f(r_{23})$ shows that this term refers to excitation of three particles having momenta $\underline{k}_1$, $\underline{k}_2$, $\underline{k}_3$ with $\underline{k}_1 + \underline{k}_2 + \underline{k}_3 = 0$. The previous cluster integral treatments do not impose this constraint of non-repeated indices in the ground state wave function. As a result, they include (but only partially) excitations of three and more particles in addition to the pair excitations. The net effect is to give an approximate expression for the ground state energy which is in the same sense as the perturbation theory calculation, and hence, not directly comparable. With the constraint of non-repeated indices, the cluster integral development becomes equivalent to the pair excitation approximation perturbation theory, and the solution of the variational problem for the pair function $f(r_{ij})$ and ground state energy yields again the same results as perturbation theory.

Prior to the demonstration of this, the cluster integral formalism is introduced and a critical review is presented of both the previous cluster integral treatments and the pair excitation perturbation theory. Then the characteristics of the ground state for Bosons with repulsive interactions is obtained by a variational method in the approximation of single pair excitations to show the connection with the perturbation theory method at an early stage. This is followed by the detailed demonstration of how the cluster integral formalism may be treated to produce results equivalent to those obtained from perturbation theory. This involves the application of the implications of the constraint of non-repeated indices.

Interest in the equivalence is not so much in presenting the cluster integral development as an alternative to the second quantization procedure; as employed in this investigation at least, the cluster integral formalism appears considerably more cumbersome, but proceeding in configuration space does have intuitive advantages, however. Of greater interest, perhaps, is the underlying reason for the possibility of making an exact asymptotic calculation for the ground state energy in the two procedures. In the second quantization formalism, the pair excitation approximation reduces the Hamiltonian operator from a complicated quadrilinear form in the plane wave creation and destruction operators to a simple bi-linear form, which can then be diagonalized by a canonical transformation to new operators. The cluster integral formalism without the equivalent of the pair approximation is also quite intractible because of the complicated nature of admissible graphs contributing to the pair distribution function. The equivalent of the pair excitation approximation, namely the restriction to non-repeated indices, selects out of the original hierarchy of graphs only certain ring integrals. These have a particularly simple structure which enables the exact evaluation of their contribution to the pair distribution function. This fact, utilized previously in, for example, the Debye-Hückel theory of electrolytes, the Kahn-Uhlenbeck treatment of the perfect Bose-Einstein gas and the Born-Green theory of liquids, here again forms the basis for the possibility of the present calculation.

CHAPTER I

INTRODUCTION

As the name implies, the quantum mechanical many-body problem is concerned with the behavior of a system of a large number of interacting particles for which quantum effects are important.

The difficulty of the many-body problem is apparent already for more than two bodies as well as for a large number. The inherent inseparability of the problem is the deterrent. Even the two-body problem is tractable only through those symmetry properties that allow its reduction to the one-body relative motion problem. For three or more interacting particles, no such simplifying feature exists, and one must resort to approximate treatments. One such approach is the Hartree-Fock approximation wherein each particle is treated as moving independently in an average potential provided by all the others. The usual Hartree-Fock approximation involves writing the N-body wave function as a product of single particle functions. Other approaches include that of normal coordinates wherein the search is for independent functions which describe the collective motion of the system. These functions depend upon the particle coordinates.

For particles which obey Fermi-Dirac statistics (Fermions), typical problems include those of nuclear matter, the finite nucleus, the electron gas, liquid helium three, etc. A group of atoms is a system of particles obeying Bose-Einstein statistics (Bosons) for which investigation of quantum effects is important. It is truly a "quantum liquid" despite expectations to the contrary. The weak nature of the attractive forces between the closed shell atoms would lead to the suspicion that the helium four atom could be closely approximated by the classical hard sphere. Its behavior, however, is very different from that expected from a classical system of hard spheres. Included among its properties is that of superfluidity (1) (2) (3).

Landau's (4) explanation of the thermodynamic properties of liquid helium four in terms of elementary excitations was justified by Feynman (5). To do this, Feynman used a wave-function which was dependent upon knowledge of the liquid structure factor empirically. This phenomenological foundation for the theory of the thermodynamic properties can only be overcome by solving the Schrödinger equation to determine the energy eigenvalues and the eigenfunctions for the system. This is one reason for interest in this particular type of the quantum mechanical many-body problem, namely that of a system of a large number of strongly interacting Bosons. With the eventual aim of understanding liquid helium four, a number of such systems with various characteristics have been studied.

The properties of a Boso system of particles with repulsive interactions using the formalism of second quantization has been treated by several investigators. In particular, Boguliubov and Zubarev (6)(7)(8) have considered this problem in the limit of weak coupling, i.e. weak repulsive forces. An important contribution from this work was that a finite fraction of particles in the ground state causes a linearization of the Hamiltonian in first approximation. Lee, Huang, and Yang (9) (10) have used the method of pseudopotentials to consider the case of a dilute collection of hard spheres. Brueckner and Sawada (11) consider the problem for a less dilute system (i.e. at higher densities) using the "Brueckner t-matrix" method. This procedure obtains the actual wave function by operating with the t-matrix operator on the wave function for the ideal Boson gas, i.e. plane waves. More recently (12) (13) the same problem has been considered dealing directly with the wave function in configuration space, using the theory of cluster expansions first introduced in statistical mechanics (14). In these latter treatments the ground state wave function is expressed as a product of pair functions. The problem of evaluating the expectation value for the energy then becomes analogous to evaluating the classical partition function for an imperfect gas, expressed in terms of Mayer's cluster integrals. By considering only contributions to the energy from ring integrals, a tractable expression for the ground state energy is obtained. Then a choice for the pair function is made and subsequent variation with respect to a parameter in this trial function has been shown to yield a ground state energy quite close to the exact asymptotic expression obtained in the work of Lee, Huang, and Yang and Brueckner and Sawada mentioned above where the contribution to the energy from pair excitations was calculated exactly.

Now one might naturally ask how this cluster integral method in configuration space is related to the perturbation theory calculation using momentum-space eigenfunctions. An analogous situation exists for the calculation of the partition function of an ideal Bose gas, where there is a cluster integral development which is completely equivalent to the more usual sum-over-states (15). One might expect that here as well, the pair approximation perturbation theory should have its exact counterpart in a configuration space cluster integral development. The purpose of the present work is to show that this expectation is indeed fulfilled. The cluster integral calculations previously made are not directly comparable to the perturbation calculations simply because the class of ring integrals which were taken as contributing to the ground state energy do not correspond to the pair approximation of perturbation theory.

In Chapter II, the formalism of the cluster development is introduced and the details of the previous ring integral treatments are discussed. The important approximation which allowed an exact perturbation theory calculation in the pair approximation is briefly recalled and its implications for the cluster method are discussed.

In Chapter III, the connection between the perturbation theory calculation in the pair approximation and the cluster expansion method is demonstrated.

CHAPTER II

CLUSTER EXPANSIONS AND THE GROUND STATE OF BOSONS WITH REPULSIVE INTERACTIONS

The approach used to investigate the properties of the ground state of a system of Bosons will be a variational one. In particular, interest will be centered on the ground state energy and the variational effort will be toward obtaining the best approximation to it. The ground state energy will be obtained by variation of the expectation value of the Hamiltonian,

$$\langle H \rangle = \frac{\int \Phi^* \left[-\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j=1}^{N} V(r_{ij}) \right] \Phi \, dr^N}{\int \Phi^* \Phi \, dr^N} \tag{1}$$

where $dr^N = dr_1 \, dr_2 \ldots dr_N$. In this expression for $\langle H \rangle$, it is assumed that the interaction energy $V(r^N)$ may be expressed as the indicated sum of pair interactions. Furthermore, the system under consideration is a system of N non-relativistic Boson particles contained in a volume V. Interest will eventually be centered on the case $N \to \infty$ and $V \to \infty$ but $N/V = \rho$ remains finite.

The ground state wave function Φ will be written in the form

$$\Phi = \prod_{i<j=1}^{N} \psi(r_{ij}) = \prod_{i<j=1}^{N} \left[1 + f(r_{ij}) \right] . \tag{2}$$

The use of this particular form for the ground state wave function for Bosons with repulsive interactions seems to have been first suggested by N. F. Mott and used by R. B. Dingle (1). It was subsequently used in a cluster development for the expectation value of the energy by R. Jastrow (2). It should be noted that such a product of two-body wave functions is necessary to describe hard-sphere interactions. A product of single particle wave functions will not vanish inside a hard core, i.e. for $V(r_{ij}) = \begin{cases} 0 & r_u > a \\ \infty & r_{ij} \leq a \end{cases}$, $\Phi(r_1..r_N)$ must equal zero whenever $r_{ij} \leq a$.

The pair function $\psi(r_{ij})$ or $f(r_{ij})$ will be determined by the variation of the expectation value of the Hamiltonian, i.e. the variation of equation (1) with ψ the trial function of equation (2).

<u>General Cluster Formulation.</u>--To apply the cluster expansion techniques to this problem, it is necessary to rewrite the expectation value of the Hamiltonian in a suitable form. Using equation (2) for Φ in equation (1),

$$\langle H \rangle = \frac{\int \prod_{i<j=1}^{N} \psi(r_{ij}) \left[-\frac{h^2}{2m} \sum_k \nabla_k^2 + \sum_{\ell<m=1}^{N} V(r_{\ell m}) \right] \prod_{i<j=1}^{N} \psi(r_{ij}) dr^N}{\int \prod_{i<j=1}^{N} \psi^2(r_{ij})\, dr^N} \tag{3}$$

Define the quantities

$$K_{\ell m} = \prod_{\substack{i<j=1 \\ (ij) \neq (\ell m)}}^{N} \psi(r_{ij}) \tag{4}$$

and

$$c(r_{12}) = \frac{N(N-1)}{\rho^2} \frac{\int K_{12}^2 \quad d\underline{r}_3 \cdots d\underline{r}_N}{\int \prod\limits_{i<j=1}^{N} \psi^2(r_{ij}) d\underline{r}^N} \tag{5}$$

$$= \frac{N(N-1)}{\rho^2 \, \psi^2(r_{12})} \frac{\int \prod\limits_{i<j=1}^{N} \psi^2(r_{ij}) d\underline{r}_3 \cdots d\underline{r}_N}{\int \prod\limits_{i<j=1}^{N} \psi^2(r_{ij}) d\underline{r}_1 \cdots d\underline{r}_N}$$

Then

$$\rho^2 \, \psi^2(r_{12}) \; c(r_{12}) = N(N-1) \; P(\underline{r}_1, \underline{r}_2) = n(\underline{r}_1, \underline{r}_2) \tag{6}$$

where $P(\underline{r}_1, \underline{r}_2) \, d\underline{r}_1 \, d\underline{r}_2$ is the probability that particles one and two are simultaneously in the volume elements $d\underline{r}_1, d\underline{r}_2$ centered on $\underline{r}_1$ and $\underline{r}_2$ respectively. The quantity $n(\underline{r}_1, \underline{r}_2)$ is the quantum mechanical analogue of the classical pair distribution function. $\langle H \rangle$ is now written as the sum of $\langle T \rangle$ and $\langle V \rangle$ and

$$\langle V \rangle = \frac{\int \prod\limits_{i<j=1}^{N} \psi(r_{ij}) \sum\limits_{k<m=1}^{N} V(r_{ij}) \prod\limits_{i<j=1}^{N} \psi(r_{ij}) d\underline{r}^N}{\int \prod\limits_{i<j=1}^{N} \psi^2(r_{ij}) d\underline{r}^N} \tag{7}$$

is examined first. As it consists of the indicated sum over pairs and the $N(N-1)/2$ integrals involved are all of the same value then,

$$\frac{\langle V \rangle}{N} = \frac{\rho^2}{2} \int V(r_{12}) \; \psi^2(r_{12}) \; C(r_{12}) d\underline{r}_1 \; d\underline{r}_2 \tag{8}$$

Transforming to the variables $\underline{r}_1$ and $\underline{r}_{12}$, this becomes

$$\langle V \rangle = \frac{\rho}{2} \int V(r_{12}) \; \psi^2(r_{12}) \; C(r_{12}) \; d\underline{r}_{12} \tag{9}$$

If

$$\langle T\rangle = \frac{-\frac{\hbar^2}{2m}\int \prod_{i<j=1}^{N} \psi(r_{ij}) \left[\sum_k \nabla_k^2\right] \prod_{i<j=1}^{N} \psi(r_{ij})\, d\underline{r}^N}{\int \prod_{i<j=1}^{N} \psi^2(r_{ij})\, d\underline{r}^N} \tag{10}$$

may also be written as a sum over pairs, a similar reduction to that for $\langle V\rangle$ may be effected. Noting that

$$\underline{\nabla}_k \prod_{\ell<n=1}^{N} \psi(r_{\ell n}) = \sum_{n\ 1}^{N} \left[\nabla_k \ \psi(r_{\ell n})\right] k_{\ell n} \tag{11}$$

and hence

$$\nabla_k^2 \prod_{\ell<n=1}^{N} \psi(r_{\ell n}) = \sum_{\ell<n=1}^{N} \left\{\left[\nabla_k^2 \ \psi(r_{\ell n})\right] k_{\ell n} + \underline{\nabla}_k \ \psi(r_{\ell n})\cdot\nabla_k \ k_{\ell n}\right\} \tag{12}$$

Summing over k and interchanging the order of the summation,

$$\sum_{k=1}^{N} \nabla_k^2 \prod_{\ell<n=1}^{N} \psi(r_{\ell n}) = \sum_{\ell<n=1}^{N} \left\{\sum_k \left[\nabla_k^2 \ \psi(r_{\ell n})k_{\ell n} + \underline{\nabla}_k\psi(r_{\ell n}) \underline{\nabla}_k \ k_{\ell n}\right]\right\} \tag{13}$$

However, $\nabla_k\,(r_{\ell n}) = 0$ unless $k = \ell$ or $k = n$, so

$$\sum_{k\ 1}^{N} \nabla_k^2 \prod_{\ell<n=1}^{N} \psi(r_{\ell n}) = 2 \sum_{\ell<n=1}^{N} \left[\nabla_\ell^2 \ \psi(r_{\ell n})k_{\ell n} + \underline{\nabla}_\ell \ \psi(r_{\ell n})\cdot\underline{\nabla}_\ell \ k_{\ell n}\right] \tag{14}$$

Thus, utilizing equation (14), $\langle T\rangle$ becomes

$$\frac{\langle T\rangle}{N} = \frac{\hbar^2\rho}{2m}\int\left\{\left[\psi(r_{12})\nabla^2\psi(r_{12})\;C(r_{12})\right.\right. \tag{15}$$

$$\left.+\frac{1}{2}\;\psi(r_{12})\;\psi(r_{12})\cdot\nabla C(r_{12})\right\}\;dr_{12})$$

The expectation value for the Hamiltonian can now be written, using equations (9) and (15)

$$\frac{\langle H\rangle}{N} = \frac{\hbar^2}{4m}\int\left\{-2\left[\psi(r_{12})\nabla^2\psi(r_{12})\right]\;C(r_{12})\;-\;\frac{1}{2}\,\psi(r_{12})\;\psi(r_{12})\cdot\nabla C(r_{12})\right.$$

$$\left.+\;\frac{2m}{\hbar^2}\;V(r_{12})\;\psi^2(r_{12})\;C(r_{12})\right\}\;dr_{12} \tag{16}$$

It is now in the desired form for the use of cluster expansion techniques. $C(R_{12})$ will be expanded in a cluster expansion originally developed for the analogous two-body correlation function in classical statistical mechanics. The expansion of the classical two-body correlation function

$$F_2(1,2) = \frac{\int\cdots\int dr_3\ldots dr_N\;\;e^{-\sum\limits_{1\leq i<j\leq N}\frac{U(r_{ij})}{kT}}}{V^{N-2}\;\;Q_N} \tag{17}$$

in powers of the density is well known (18) (19). In equation (17), $U(r_{ij})$ is the two-body interaction and the configuration integral Q_N is given by

$$Q_N\;=\;V^{-N}\;\int dr_1\ldots dr_N\;e^{-\frac{1}{kT}\sum\limits_{1\leq i<j\leq N}U(r_{ij})} \tag{18}$$

The expansion is made under the assumption that N, $V \rightarrow \infty$, but $N/V = \rho$ remains finite. $C(r_{12})$ is suitable for a cluster expansion in powers of the density

$$C(r_{12}) = 1 + \sum_{n=1}^{\infty} \rho^n \xi_n (r_{12}) \tag{18}$$

where

$$\xi_n (r_{12}) = \frac{1}{n!} \int_V \sum^{(n)} \prod h(r_{ij}) \, d\underline{r}_3 \ldots d\underline{r}_{n+2} \tag{19}$$

$$h(r_{ij}) = \psi^2(r_{ij}) - 1 = 2f(r_{ij}) + f^2 (r_{ij})$$

and the integrand $\sum^{(n)} \prod h(r_{ij})$ indicates the sum of all connected products for which each particle of the set n is connected to particles one and two by an independent path. $\xi_n(r_{12})$ is often called a "general 1,2-irreducible cluster integral" (19). An alternate prescription for $\sum^{(n)} \prod h(r_{ij})$ is that $\sum^{(n)}$ indicates summation over all possible "general 1,2-irreducible" cluster diagrams that can be formed with the singled out points one and two plus n-given field points. A"general 1,2-irreducible" cluster diagram with n-given field points is one in which each of the on-given points lies on at least one continuous path going from one to two without passing any point more than once (19). The link connecting i and j corresponds to the function $h(r_{ij})$. "General 1,2-irreducible cluster diagrams" are illustrated in Figure 1 for (a) n = 1, (b) n = 2 and (c) n = 3. A number of these cluster diagrams differ in the ordering of the field particles but lead to integrals of the same numerical

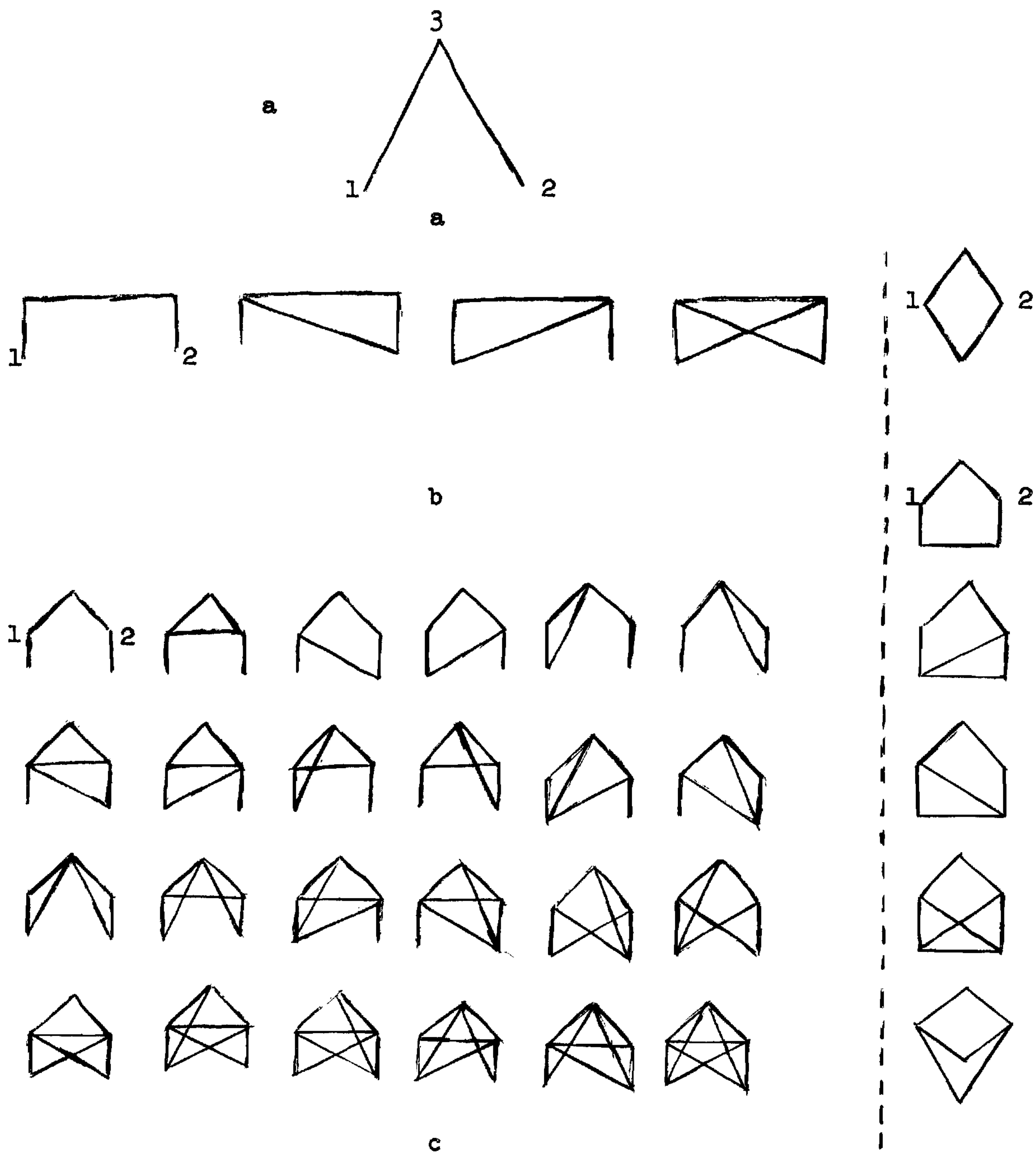

Figure 1. General 1,2 Irreducible Cluster Diagrams

(a) n = 1 (b) n = 2 (c) n = 3

value. To illustrate the procedure, the diagrams and the corresponding integrals will be examined for n = 1 and n = 2. For n = 1 (See Figure 1(a).)

$$\xi_1(r_{12}) = \frac{1}{1!}\int dr_3 \; h(r_{13}) \; h(r_{32}) \; . \tag{20}$$

For n = 2 (See Figure 1(b).)

$$\xi_2(r_{12}) = \frac{1}{2!}\int dr_3 dr_4 \Big\{ h(r_{13}) h(r_{34}) h(r_{42}) \big[2 + 4h(r_{14}) + h(r_{14}) h(4_{23}) \big] + h(r_{13}) h(r_{32}) h(r_{14}) h(r_{24}) \Big\} \tag{21}$$

or

$$\xi_2(r_{12}) = \frac{1}{2!}\int dr_3 dr_4 \; h(r_{13}) h(r_{34}) h(r_{42}) \big[2 + 4h(r_{14}) \; h(r_{14}) h(r_{23}) \big] + 1/2 \,! \; \big[\xi_1(r_{12})\big]^2 \tag{22}$$

An alternate cluster expansion of $C(r_{12})$ may be made in terms of the "simple 1,2-irreducible" cluster integrals (19). Expressed in terms of these, the function $C(r_{12})$ is

$$C(r_{12}) = \exp\left\{ - \sum_{\ell=1}^{\infty} \beta_\ell \, (r_{12}) \, \rho^{\ell} \right\} \tag{23}$$

where

$$\beta_\ell \, (r_{12}) = \frac{1}{\ell!} \int \sum_{s}^{(\ell)} \prod h(r_{ij}) \; d\underline{r}_3 \ldots d\underline{r}_{\ell+2} \tag{24}$$

where $\sum s^{(\ell)} \prod h(r_{ij})$ indicates summation over all possible "simple 1,2-irreducible" cluster diagrams that can be formed with the singled-out points one and two plus ℓ-given field points. A simple irreducible cluster diagram is a "general 1,2-irreducible" cluster diagram with -given field points with the restriction that there is at least one continuous path passing through neither point one nor point two and joining any two field points. In the illustrated "general 1,2-irreducible cluster diagrams" for the cases n = 1,2, and 3 in Figure 1, the diagrams to the left of the dotted lines in each case are "simple 1,2-irreducible cluster diagrams."

Using the expansion given in equation (23) for $C(r_{12})$ in equation (15), the expectation value for the energy became

$$\langle H\rangle = -\frac{\hbar^2\rho}{2m}\int\Bigg[\psi\,\nabla^2\psi\;\exp\left\{-\sum_{n=1}^{\infty}\rho^n\beta_n(r_{12})\right\} + \frac{1}{2}\,\psi\nabla\psi\cdot\nabla\exp\left\{-\sum_{n=1}^{\infty}\rho^n\beta_n(r_{12})\right\} - \frac{m}{\hbar^2}V(r_{12})\;\psi^2\exp\left\{-\sum_{n=1}^{\infty}\rho^n\beta_n(r_{12})\right\}\Bigg]d\underline{r}_{12} \tag{25}$$

or

$$\langle H\rangle = -\frac{h^2\rho}{2m}\int\left\{\psi\,\nabla\psi^2 - \frac{1}{2}\psi\nabla\psi\left[\sum_{n=1}^{\infty}\rho^n\,\nabla_1\,\beta_n(r_{12})\right] - \frac{m}{\hbar^2}\;\psi^2\,r_{12}\right\}\exp\left[-\sum_{n=1}^{\infty}\rho^n\,\beta_n(r_{12})\right]d\underline{r}_{12}\,. \tag{26}$$

The above represents an alternate expression for $\langle H \rangle$ to that in equation (15). There are thus two cluster expansions which may be used for $C(r_{12})$, namely those of equation (18) and equation (23). The expansion of equation (18) was used in the work of Aviles (20) which will be discussed in the next section. Its use in the next chapter is explained by the requirements imposed there.

The variation of $\langle H \rangle$, given in equation (1) for $\Phi(\underline{r}^N)$ will yield the Schrodinger equation. The variation of $\frac{\langle H \rangle}{N}$, given in equation (16) with respect to $\psi(\underline{r}_{12})$ yields the Euler equation:

$$\nabla^2 \psi(\underline{r}) + \frac{2m}{\hbar^2} \left\{ U(\underline{r}) - 1/2V(\underline{r}) \right\} \psi(\underline{r}) = 0 \tag{27}$$

where for $C(\underline{r}) \neq 0$,

$$\frac{2m}{\hbar^2} U(r) = \frac{4 \nabla C_{(r)} (\nabla \psi(\underline{r})) - \psi(r) \left\{ 2 \nabla^2 \psi(r) + \frac{2m}{\hbar^2} V(r) \psi(r) - \nabla\psi(r) \nabla \right\} \frac{\partial C(r)}{\partial \psi(r)} \nabla^2 C}{4C(\underline{r}) \psi(r)} \tag{28}$$

and $C(\underline{r}_{12})$ is given by either equation (18) or equation (23).

This Euler equation for the two-body wave function $\psi(\underline{r}_{12})$ is similar to the Schrodinger equation for two particles in a potential $1/2V(\underline{r}) - \frac{2m U}{\hbar^2}(r)$ The "effective potential" $U(r)$ represents the effect upon the pair of particles under consideration of the remaining p N-2 particles.

<u>The Approach of Jastrow and Aviles</u>.--With the expectation value for the Hamiltonian in the desired form for the use of cluster expansion techniques, and presented by equation (16), it is necessary to recognize that the problem in its present form is still somewhat intractable. The variation of

$\frac{\langle H \rangle}{N}$ with respect to $\psi(r_{12})$ yielded the Euler equation of equation (27), $\nabla^2 \psi(r) + \frac{2m}{\hbar^2} \left\{ U(r) - 1/2V(r) \right\} \psi(r) = 0$ where the "effective potential" $U(r)$ is given by equation (28). The solution of this equation yields the minimizing $\psi(r)$. One method of solution of this equation is by iteration, i.e. start with some approximate $\psi(r)$, say $\psi_o(r)$ which satisfies the boundary conditions the $\psi(r)$ must satisfy and insert it into $U(r)$. Call this $U(r)$, $U_o(r)$ and solve equation (27), for $\psi(r)$ with $U(r)$ replaced by $U_o(r)$. This solution will be called $\psi_1(r)$. Repeat the preceding process. This will generate a sequence of $\psi_i(r)$. If the process is convergent, there will eventually be a $\psi_k(r)$ such that $\psi_k(r) = \psi_{k+1}(r)$. Then $\psi_k(r)$ will be the solution of the integro-differential equation. One difficulty with this procedure is that the calculation of $U(r)$ involves the function $C(r)$. For the procedure to be other than purely formal, it must be known whether $C(r)$ in terms of the series prescription of equation (18) is convergent for every $\psi_i(r)$. Even formally, the calculation of the cluster integrals $\xi_j(r_{12})$ is quite difficult for most prospective $\psi_i(r)$.

Instead of proceeding directly to obtain $\psi(r)$ and the minimal $\frac{\langle H \rangle}{N}$ by a direct variation of $\frac{\langle H \rangle}{N}$, Jastrow (21) suggested as a first approximation the use of a trial function $\psi_o(r)$. This function would satisfy the boundary conditions expected of $\psi(r)$ and would contain a single variable parameter. Instead of being used, as in the procedure just discussed as a first iterate of the variational equation, it would be inserted in the expression for $\frac{\langle H \rangle}{N}$ and variation would be made with respect to its parameter. For the hard-sphere interaction, Jastrow used as his single-parameter trial two-body wave function

$$\psi_0(r) = \begin{cases} 0 \quad , & r < a \\ 1 - \frac{a}{r}\, e^{-\varepsilon(r-a)}, & r \geq a \end{cases}$$

where a is the hard sphere diameter and ε is the parameter. It should be noted that this function vanishes inside the core and approaches one for large R.

For the problem of dilute hard sphere bosons, Jastrow made the further approximation, although unordered arbitrary and with uncontrolled error, that

$$C(r_{12}) = 1 \quad . \tag{30}$$

From the viewpoint of the cluster expansions, they were terminated after the first term. In terms of the definition of $C(r_{12})$, one has from equation (16) that

$$P(\underline{r}_1,\underline{r}_2)\ d\underline{r}_1 d\underline{r}_2 = \frac{\psi^2(r_{12})\ C(r_{12})}{V^2}\ d\underline{r}_1 d\underline{r}_2 \tag{31}$$

where $P(\underline{r}_1,\underline{r}_2)\ d\underline{r}_1 d\underline{r}_2$ is the probability that particles one and two are simultaneously in the volume elements $d\underline{r}_1$, $d\underline{r}_2$ centered on $\underline{r}_1$ and $\underline{r}_2$ respectively. For $C(\underline{r}_{12}) = 1$,

$$P(\underline{r}_1,\underline{r}_2)\ d\underline{r}_1 d\underline{r}_2 = \frac{\psi^2(r_{12})}{V^2}\ d\underline{r}_1\ d\underline{r}_2 \ .$$

Thus, for $r_{12} < a$,

$$P(\underline{r}_1,\underline{r}_2)\ d\underline{r}_1\ d\underline{r}_2 = 0 \ .$$

But for $r_{12} > a$, $P(\underline{r}_1,\underline{r}_2)$ is not affected by the presence of the other particles, except as they influence $\psi(r_{12})$.

With $C(r_{12}) = 1$, equation (16) for $\frac{\langle H \rangle}{N}$ becomes

$$\frac{\langle H \rangle}{N} = \frac{\rho\hbar^2}{4m} \int \left\{ -2\, \psi(r)\, \nabla^2 \psi\,(r) + \frac{2m}{\hbar^2}\, V(r)\, \psi^2(r) \right\} d\underline{r} \tag{32}$$

Note that this eliminates the troublesome $\nabla\psi \cdot \nabla C$ term. For the hard sphere interaction and the spherically-symmetric $\psi_o(r)$, this becomes

$$\frac{\langle H \rangle}{N} = \frac{\rho\hbar^2}{2m} \int_a - \psi_o(r)\, \nabla^2\, \psi_o(r)\, \left[4\pi r^2\ dr\right]$$

For the $\psi_c(r)$ of equation (29), $\psi_o(r) = 1 - \frac{a}{r}\ e^{-\varepsilon(r-a)}$, equation (33) becomes

$$\frac{\langle H \rangle}{N} = \frac{4\pi\rho h^2}{2m} \int (-a\varepsilon^2) \left[- \frac{e^{-\varepsilon(r-a)}}{r} + \frac{ae^{-2\varepsilon(r-a)}}{r^2} \right] r^2 dr \tag{34}$$

or

$$\frac{\langle H \rangle}{N} = \frac{4\pi\, \rho\, ah^2}{2m} \quad \varepsilon^2 \int_a^\infty \left[re^{-\varepsilon(r-a)} - ae^{-2\varepsilon(r-a)}\right] \quad dr \tag{35}$$

Integrating, one has for $\varepsilon \neq 0$,

$$\frac{\langle H \rangle}{N} = \frac{4\pi\, \rho\, a\hbar^2}{2m} \quad \left[1 + \frac{a\varepsilon}{2}\right] . \tag{36}$$

Examining equation (36), one sees that the minimal value of $\frac{\langle H \rangle}{N}$ occurs for $\varepsilon = 0$, i.e.

$$\frac{\langle H \rangle}{N} = \frac{4\pi\, \rho\, a\hbar^2}{2m} . \tag{37}$$

However, equation (36) was calculated for $\varepsilon \neq 0$. For $\varepsilon = 0$,

$$\int_a^\infty \psi_o \nabla^2 \psi_o r^2 \, dr = 0 .$$

This contradiction is resolved if one realizes that the correct expression for the kinetic energy is $\frac{\hbar^2}{2m} \int \left|\nabla\psi\right|^2 d\underline{r}^N$ and that the transformation to $-\frac{\hbar^2}{2m} \int \psi \nabla^2 \psi \; d\underline{r}^N$ was invalid for $\varepsilon = 0$, and hence $\psi = 1$ outside the core. Evaluation of $\int_a^\infty \left| \nabla \psi_o \right|^2 r^2 \, dr$ leads to

$$\frac{\langle H \rangle}{N} = \begin{cases} 4\pi \rho a \frac{\hbar^2}{2m} \left\{ 1 + \frac{a\varepsilon}{2} \right\}, & \varepsilon \neq 0 \\ 4\pi \rho a \frac{\hbar^2}{2m} & , \varepsilon = 0 \end{cases} \tag{38}$$

Thus the previous conclusion that the minimal value of $\frac{\langle H \rangle}{N}$ in this approximation is $4\Pi\rho a \frac{\hbar^2}{2m}$ (the Lenz term (22)) and occurs for $\varepsilon = 0$, is true.*

Aviles (25) extended the work of Jastrow by including more terms of the cluster expansion of $C(r_{12})$. In particular, from the cluster expansion given by equation (18) and equation (19), only the set of cluster integrals arising from those diagrams which are chain connected are included. As illustrated in Figure 2, for arbitrary order m, they have neither internal connections nor more than one path leading from particles one or two. For the illustrated set m, the cluster integral is

$$\xi_{m,\text{ chain}} = \frac{1}{m!} \int m! \; h(r_{13}) h(r_{34}) \ldots h(r_{m+2}2) \; d\underline{r}_3 d\underline{r}_4 \ldots d\underline{r}_{m+2} \tag{39}$$

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*Jastrow reported the minimizing value to be $4\pi(\rho a^3)^{1/2}$ (23).

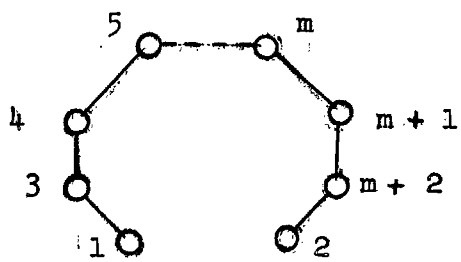


Figure 2. Ring Cluster Diagram of Order m

Define the Fourier transform of $h(\underline{r})$ as

$$\varphi(k) = \int h(\underline{r})\, e^{-i\underline{k}\cdot\underline{r}}\, d\underline{r}\ . \tag{40}$$

The Fourier transform of $\xi_{m,\text{chain}}\ (r_{12})$ is

$$\Gamma(k) = \int \xi_{m,\text{chain}}\ (r_{12})\ e^{-i\underline{k}\cdot\underline{r}_{12}}\ d\underline{r}_{12} \tag{41}$$

$$= \int \cdots \int h(r_{13})h(r_{34})\ldots h(r_{m+2,2})\ e^{-i\underline{k}\cdot\underline{r}_{12}}\ d\underline{r}_3 d\underline{r}_4 \ldots d\underline{r}_{m+2} d\underline{r}_{12}$$

But $\underline{r}_{12} = \underline{r}_1 - \underline{r}_2$

$$= \underline{r}_1 - \underline{r}_3 + \underline{r}_3 + \underline{r}_3 - \underline{r}_4 + \underline{r}_4 + \ \cdots\ - \underline{r}_{m+2} + r_{m+2} - \underline{r}_2$$

Thus $\Gamma(k)$ becomes

$$\Gamma(k) = \int \cdots \int \left[h(\underline{r}_{13}) e^{-i\underline{k}\cdot\underline{r}13}\right] \left[h(r_{34}) e^{-i\underline{k}\cdot\underline{r}34}\right] \ldots \tag{42}$$

$$\left[h(r_{m+2,2})\ e^{-i\underline{k}\cdot\underline{r}m+2,2}\right]\ d\underline{r}_3 d\underline{r}_4\ \ldots\ d\underline{r}_{m\ 2} d\underline{r}_{12} = \left[\varphi(k)\right]^{m+1}$$

Hence

$$\xi_{m,\text{chain}}(r_{12}) = \frac{1}{(2\Pi)^3} \int \left[\varphi\,(k)\right]^{m+1}\ e^{-i\underline{k}\cdot\underline{r}12}\ d\underline{k} \tag{43}$$

The cluster expansion for the chain terms,

$$C_{\text{chain}}\ (r_{12}) = 1 + \sum_{n=1}^{\infty}\ \rho^n\ \ \xi_{n,\text{chain}}\ (r_{12}) \tag{44}$$

becomes

$$C_{chain}(r_{12}) = 1 + \frac{1}{(2\pi)^3} \sum_{n=1}^{\infty} \frac{1}{\rho} \int \left[\rho\varphi(k)\right]^{h+1} e^{-i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \tag{44}$$

Formal interchange of summation and integration yields

$$C_{chain}(r_{12}) = 1 + \frac{\rho}{(2\Pi)^3} \int \frac{\varphi^2(k)}{1-\rho\varphi(k)}\, e^{-i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \tag{45}$$

where $|\rho\varphi(k)| < |$.

Aviles makes the approximation $C(r_{12}) = C_{chain}(r_{12})$ and uses the same single parameter wave function $_o(r_{12})$ of equation (29) for the hard sphere interaction. Retaining only terms of lowest order in the parameter ε , Aviles finds for $\frac{\langle H\rangle}{N}$,

$$\frac{\langle H\rangle}{N} = 4\pi\rho a \frac{\hbar^2}{2m} \left[1 + \varepsilon\left(1 + \frac{8\pi\rho a^3}{2}\right)^{\frac{1}{2}} - \frac{\varepsilon}{1+\sqrt{1\ \ \frac{8\pi\rho a^3}{\varepsilon^2}}}\right]$$

The ε which minimizes this expression is $\varepsilon = \sqrt{\frac{8}{3}\pi\rho\ a^3}$. Thus, the minimal $\frac{\langle H\rangle}{N}$ is

$$\frac{\langle H\rangle}{N} = 4\pi\rho a \frac{\hbar^2}{2m}\left[1 + \frac{10}{9}\sqrt{6\pi}\,(\rho\, a^3)^{\frac{1}{2}}\right] .$$

Iwamoto also obtained this result (12). Comparison with the exact result of Lee, Huang, and Yang for the first two terms

$$\frac{\langle H\rangle}{N} = 4\pi\rho\, a \frac{\hbar^2}{2m}\left[1 + \frac{128}{15\sqrt{\pi}}(\rho\, a^3)^{\frac{1}{2}}\right]$$

reveals that the coefficient of the term $(\rho a^3)^{\frac{1}{2}}$ in equation (47) is larger, namely 4.824... compared with 4.814.... This leads Aviles to conclude

"The closeness of the two solutions shows that the trial function $\Phi(r^N) = \Pi\ \psi(r_{ij})$ with $\psi(r_{ij})$ given by equation (29) provides a rather accurate description of the low density behavior of the hard sphere boson system in the ground state" (25). When making such a comparison with the exact results of Lee, Huang, and Yang (26), it is important and instructive to review those facts and features which made their calculation possible.

Basic Approximation.--The crucial point in treating the system of Bose particles with repulsive interactions is that one expects a finite fraction of particles in the free particle ground state, even with the interactions turned on. This allows an essential simplification in treating the off-diagonal matrix elements of the two body interaction $V(r_{ij})$ between plane wave states expressed in terms of the occupation number representation. These matrix elements describe transitions in which two particles of moments $\underline{k}_\alpha$ and $\underline{k}_\beta$ collide and go into states $\underline{k}_\mu$ and $\underline{k}_\nu$ with $\underline{k}_\alpha + \underline{k}_\beta = \underline{k}_\mu + \underline{k}_\nu$. Its value is

$$\frac{V_{\alpha\mu}}{\Omega} \left[n_\alpha\, n_\beta\, (n_\mu + 1)(n_\nu + 1)\right]^{\frac{1}{2}} \tag{48}$$

where the n's are occupation numbers, Ω is the containing volume, and $V_{\alpha\mu} = \int V(r)\, e^{i(\underline{k}_\alpha - \underline{k}_\mu)\cdot \underline{r}}\, dr$. The largest contribution comes when two of the four momenta involved are zero, the matrix element being proportional to n_o/Ω, n_o is the number of particles in the free particle ground state, and $n_o \sim N$, the total number of particles. If only one momentum is zero, the matrix element is smaller than this by a factor of order $N^{-1/2}$, and if none of the four momenta are zero, the matrix element is smaller than this by a factor N^{-1}. Thus it is a good approximation to consider only the off diagonal elements of the interaction matrix giving the largest contribution, i.e., excitation and de-excitation of pairs of particles with equal and opposite moments. It was this approximation which enabled an exact calculation of the energy eigenvalues and eigenfunctions of the reduced Hamiltonian for hard spheres.

The equivalent approximation in configuration space will now be made. The ground state wave function is written in the form of equation (2)

$$\Phi = \prod_{i<j=1}^{N} \psi(r_{ij}) = \prod_{i<j=1}^{N} \left[1 + f(r_{ij})\right] \tag{49}$$

where the product is over all pairs and the pair function $f(r_{ij}) = f(r_{ji})$ is to be determined by variation of the expectation value of the Hamiltonian,

$$\int \Phi^* \Phi \, d\underline{r}^N \langle H \rangle = \int \Phi^* \left[-\frac{h^2}{2m} \sum_{i} \nabla_i^2 + \sum_{i<j=1}^{N} V(r_{ij}) \right] \Phi \, d\underline{r}^N \tag{50}$$

where $d\underline{r}^N = d\underline{r}_1 \, d\underline{r}_2 \ldots d\underline{r}_N$. If the interaction $V(r_{ij})$ were absent, $f(r_{ij})$ would be zero, and $\langle H \rangle = 0$, with all N particles in the free particle ground state. The spatial Fourier transform of $f(r_{ij})$.

$$f(r_{ij}) = \Omega^{-1} \sum_{\underline{k}=0} \gamma_{\underline{k}} \, e^{i\underline{k}\cdot(\underline{r}_i - \underline{r}_j)} \underset{\Omega \to \infty}{\longrightarrow} \frac{1}{(2\pi)^3} \int \gamma(k) e^{i\underline{k}\cdot(\underline{r}_i - \underline{r}_j)} d\underline{k} \tag{51}$$

shows that the momenta of the pair (i,j) are equal and opposite. The expanded product for Φ yields

$$\Phi = 1 + \sum_{i<j} f(r_{ij}) + \sum_{i<j} \sum_{k<\ell} f(r_{ij})\, f(r_{k\ell}) + \cdots \qquad (52)$$

The terms in this expansion refer successively to all particles in the ground state, excitation of single pairs, and, in keeping with the crucial approximation, the succeeding terms should represent multiple excitation of pairs, each pair having equal and opposite moments. This will not be true, however, unless in equation (49) all terms with any index repeated are omitted. The Fourier transform of a term with one repeated index, such as $f(r_{12})\, f(r_{23})$ shows that this term refers to excitation of three particles with $\underline{k}_1 + \underline{k}_2 + \underline{k}_3 = 0$ (27). Since this corresponds to the neglected class of off diagonal elements of the interaction matrix, these terms must be omitted, and the ground state wave function taken as

$$\Phi = \prod_{i<j=1}^{N}{}' \left(1 + f(r_{ij})\right) \qquad (53)$$

the prime denoting omission of all repeated indices.

As this discussion indicates, the cluster integral calculations previously made are not directly comparable to the perturbation theory calculations simply because the class of ring integrals which were taken as contributing to the ground state energy do not correspond to the pair approximation of perturbation theory. Not imposing the constraints of non-repeated indices in the ground state wave function, causes these previous calculations to include (but only partially) excitations of three and more particles in addition to pair excitations. The net effect is to give an approximate expression for the ground state energy which is not ordered in the same sense as the perturbation theory calculations, and hence, not directly comparable.

CHAPTER III

CLUSTER EXPANSIONS AND THE GROUND STATE OF BOSONS WITH REPULSIVE INTERACTIONS: PAIR EXCITATION APPROXIMATION

The important approximation which allowed an exact perturbation theory calculation in the pair approximation will be used in this chapter to show that the cluster expansion formalism can be handled so that it is completely equivalent to the perturbation theory treatments.

Preliminary to its application in the general cluster formalism, the major contribution to the ground state energy, from single pair excitations will be evaluated by direct methods.* This treatment is formally similar to the direct evaluation of the second virial coefficient for imperfect gases (29). It has the advantage of showing the connection with the perturbation theory method at an early stage, before the full formalism of the cluster development is introduced. From this, one can already see how the cluster expansions must be handled to count only contributions from pair excitations.

<u>Direct Evaluation of the Ground State Energy: Single Pair Excitations</u>.--To evaluate $\langle H \rangle$ by direct methods, those terms representing the excitation and de-excitation of one pair, and the interaction of an excited pair with the medium formed by the unexcited particles will be counted. As shown by Brueckner and Sawada (30), these terms give the major contribution to the ground state energy, the higher order terms describing simultaneous

*A preliminary report of this calculation has been made (28).

excitation of many pairs contributing only about 4% to the energy. The contribution of these latter terms will be included in the later discussions of this chapter.

First consider the normalization integral I_N,

$$I_N = \int \Phi^* \Phi \, d\underline{r}^N \tag{54}$$

Since the pair function $f(r_{ij})$ has no zero momentum components the integral $\int f(r) d\vec{r}$ is zero. Then the normalization integral is

$$I_N = \Omega^N + \Omega^{N-1} \sum_{i<j=1}^{N} \int f^2(r_{ij}) d\underline{r}_{ij} + \Omega^{N-2} \sum_{i<j} \sum_{k<l} \int f^2(r_{ij}) \, d\underline{r}_{ij} \int f^2(r_{k\ell}) \, d\underline{r}_{k\ell} + \cdots \tag{55}$$

The terms in this series in increasing powers of $\int f^2(r) d\underline{r}$ refer successively to no pairs excited, one pair excited, two pairs excited, etc. The n^{th} term is a sum over products of n pairs with the number of terms in the sum equal to

$$\frac{N!}{(N-2n)!\,n!\,N^n} \tag{56}$$

The integral I_N is then given by

$$I_N = \Omega^N \sum_{n=o}^{N/2} \frac{N!\,x^n}{(N-2n)\,!\,n!\,N^n} \tag{57}$$

where ρ is the density, and

$$x = \frac{\rho}{2} \int f^2(r) \, d\underline{r} \tag{58}$$

For large N and Ω, I_N has the asymptotic value (31)

$$I_N = \Omega^N \left[\frac{\sqrt{1+8x} - 1}{4x}\right]^{-1} \exp\left[\frac{-N}{8x}\left(1+4x - \sqrt{1+8x}\right)\right] \qquad (59)$$

For $x \ll 1$, this reduces to

$$I_N = \Omega^N \; e^{Nx} \qquad (60)$$

The indicated exponential dependence of the normalization integral will be cancelled by a similar factor in the kinetic and potential energy integrals. Thus the energy expectation value for the N particle system will be proportional to N (as of course it must).

Next consider the kinetic energy integral I_T,

$$I_T = \frac{-Nh^2}{2m}\int \Phi^* \nabla_1^2 \; d\underline{r}^N \qquad (61)$$

With the ground state wave function given by equation (53), this becomes

$$I_T = \frac{-Nh^2}{2m}\left\{\sum_{i<j} f(r_{ij})\nabla_1^2 f(r_{ij})d\underline{r}^N + \sum_{i<j}\sum_{k<\ell}\int f(r_{ij})f(r_{k\ell}) \nabla_1^2 f(r_{ij})f(r_{k\ell})d\underline{r}^N + \dots\right\} = \frac{-Nh^2}{2m}\int f(r)\nabla^2 f(r)d\underline{r} \sum_{n=1}^{N/2} C(n)\,\Omega^{N-n} \left[\int f^2(r)\,dr\right]^{n-1} \qquad (62)$$

where $C(n)$ is the number of ways of writing the product of n functions $f(r^{st})$ such that no index appears twice and index number 1 appears once,

$$C(n) = \frac{(N-1)!}{(N-2n)!\,(n-1)!\,2^{n-1}}$$

Terms containing $\int \nabla^2 f(r)d\underline{r}$ are zero, since $f(r)$ has no zero-momentum components, and therefore do not appear in equation (62). Then the kinetic energy integral is

$$I_T = \frac{-N\hbar^2}{2m} \; \Omega^N \; \rho \int f(r)\, \nabla^2 f(r) d\underline{r} \sum_{n=1}^{N/2} \frac{(N-1)! \; x^{n-1}}{(N-2n)! \; (n-1)! \; N^n} \tag{64}$$

For large N and small x, the sum goes like e^{Nx}, but dividing by the normalization integral gives a kinetic energy proportional to the total number of particles.

$$\langle T\rangle = \frac{I_T}{I_N} = \frac{-\hbar^2 \rho}{2m} \int f(r) \nabla^2 f(r) d\underline{r} \frac{\partial}{\partial x} \; \log \sum_{n=o}^{N/2} \frac{N! \; x^n}{(N-2n)!\, n! \; N^n}$$

$$= \frac{-N\hbar^2 \rho}{2m} \int f(r)\, \nabla^2 f(r) d\underline{r}. \tag{65}$$

The integral for the potential energy is

$$I_V = \frac{N(N-1)}{2} \int \Phi^* \, V(r_{12}) \, \Phi \, d\underline{r}^N \tag{66}$$

In its evaluation the following types of contributions to the energy are encountered. First there is the integral $\int V(r_{12}) \; d\underline{r}_1 \; d\underline{r}_2$. This represents interaction between the unexcited pair (1,2) and is represented graphically in figure 3(a) . Next is the integral $\int V(r_{12}) f(r_{12}) d\underline{r}_1 \; d\underline{r}_2$, represented by (b) in Figure 3 . This term refers to excitation and deexcitation of the pair (1,2) from or to the free particle ground state. In Figure 3(c) is shown the diagram for the integral $\int f(r_{12}) V(r_{12}) f(r_{12}) d\underline{r}_1 d\underline{r}_2$, representing the interaction between the excited pair (1,2). This term can be neglected since one can show that in the final result, it contributes to the energy in a higher order. Figure 3(d) represents the integral $\int f(r_{1j}) V(r_{12}) f(r_{2j}) d\underline{r}_1 \; d\underline{r}_2 \; d\underline{r}_j$. This describes interaction of an excited pair (say 1,j) with one particle, 2, in the "medium" of unexcited particles, resulting in de-excitation of 1 and excitation of 2 into the pair (2,j).

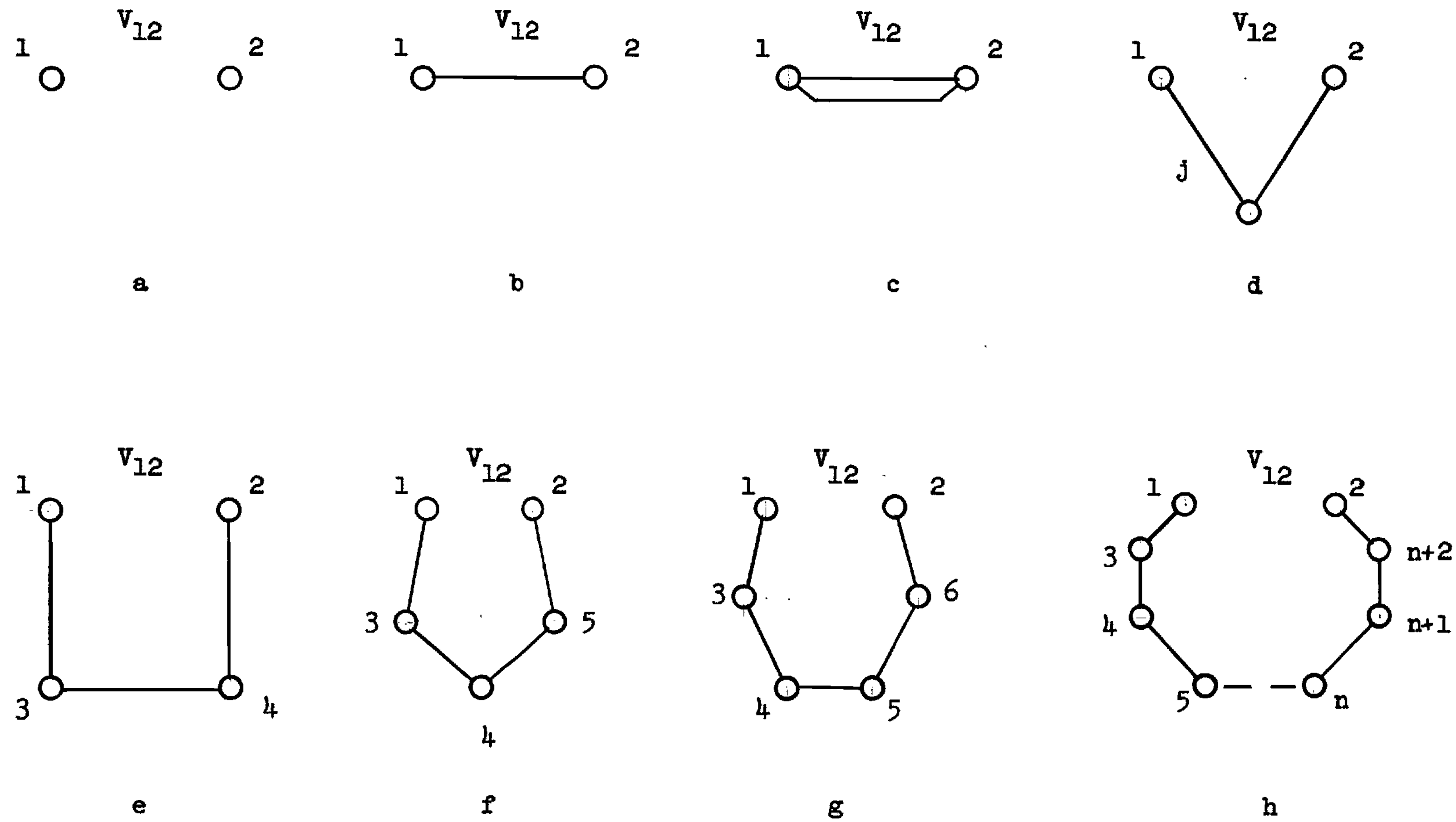


Figure 3. Graphs Representing Successive Contributions to the Ground State Energy

In the subsequent variation of $\langle H \rangle$ with respect to $f(r_{ij})$, this term provides an effective potential due to interaction of a pair through the medium of unexcited particles. In Figure 3(e) to (h) are represented terms which will be neglected in this direct calculation, but included in the general ring cluster integral method in the next section. The first of these represents the contribution to the energy from the transition from one excited pair to two excited pairs. The next represents the interaction of the two excited pairs with the medium. Figure 3(g) represents the excitation from two to three pairs, etc. The evaluation of $\langle V \rangle$, the expectation value of the potential energy from the terms indicated above is straightforward. Details are given in Appendix A. The result is

$$\langle V \rangle = \frac{N\rho g}{2} + N\rho \int V(r) f(r) d\underline{r} + N\rho^2 \int f(r') V(r) f(|\underline{r}+\underline{r}'|) d\underline{r}\, d\underline{r}' \quad (67)$$

where $g = \int V(r) d\underline{r}$. Supposing $V(r)$ is of short range, one can approximate the last integral representing interaction of excited pairs with the medium,

$$\int f(r')\, V(r) f(|r+r'|) d\underline{r}\, d\underline{r}' \cong g \int f^2(r) d\underline{r} \quad (68)$$

For the total energy, the expectation value is

$$\langle H \rangle = \frac{N\rho g}{2} - \frac{N\rho h^2}{2m} \int f(r) \nabla^2 f(r) d\underline{r} + N\rho \int V(r) f(r) d\underline{r} + N\rho^2 g \int f^2(r) d\underline{r} \quad (69)$$

Variation with respect to $f(r)$ yields

$$\frac{-\hbar^2}{2m} \nabla^2 f + \rho g f = \frac{-V(r)}{2} \quad (70)$$

and

$$\langle H \rangle = \frac{N\rho g}{2} + \frac{N\rho}{2} \int V(r)\ f(r) d\underline{r} \quad (71)$$

These results may be applied to the case of hard spheres if one utilizes the concept of the pseudopotential, introduced, in this connection by Lee, Huang, and Yang (32), and discussed in Appendix D. Here it is essential, in order to remove spurious infinities, to use the correct pseudopotential,

$$V(r) = g\,\delta(\underline{r})\,\frac{\partial}{\partial r}\,(r), \quad g = \frac{4\pi a\hbar^2}{m} \tag{72}$$

where a is the hard sphere diameter. Actually, one can use the form $V(r) = g\,\delta\,(\underline{r})$, and switch to the correct form given in equation (72) at the end of the calculation. Then the solution of equation (70) is given by

$$f(r) = -\frac{a}{r}\ \exp\left[-\sqrt{8\pi\rho a}\ \ r\right] \tag{73}$$

and the ground state energy, from equation (71) is

$$E_o = \langle H \rangle = \frac{2\pi N\rho a h^2}{m}\left[1 + \sqrt{8\pi}\ \ (\rho a^3)^{\frac{1}{2}}\right] \tag{74}$$

This is the same result that follows from perturbation theory if only the excitation of single pairs is counted (33). The multiple pair excitations so far neglected will be included in the following section in which the ground state energy is obtained as

$$E_o = \frac{2\pi N h^2 \rho a}{m}\left[1 + \frac{128}{15\sqrt{\pi}}\ \ (\rho\, a^3)^{\frac{1}{2}}\right] \tag{75}$$

This is the result previously obtained from perturbation theory (34), (35). Comparison of equation (22) with equation (21) confirms the remark, made earlier in this section, that the single pair excitations make a contribution of 96% to the coefficient of the second term in the asymptotic expansion of the ground state energy.

The Fourier transform of $f(r)$, which from equation (51) is given by

$$\gamma(k) = \int f(r)\, e^{-i\underline{k}\cdot\underline{r}}\, d\underline{r} = \frac{-4\pi a}{k^2 + 8\pi a \rho} \tag{76}$$

is the probability amplitude for an excited pair of momentum $\underline{k}$ and $-\underline{k}$, and through the factor $8\pi a\rho$ in the denominator, includes the interaction of the single excited pair with the medium.

Multiple Pair Excitations.--The aim now is to evaluate the ground state energy by variation of $\langle H\rangle$, the expectation value for the Hamiltonian of the Bose system of N interacting particles, given by equation (1)

$$\langle H\rangle = \frac{\int \Phi^* \left[\frac{-\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j=1}^{N} V(r_{ij})\right] \Phi\, d\underline{r}^N}{\int \Phi^* \Phi\, d\underline{r}^N}$$

where $d\underline{r}^N = d\underline{r}_1 \ldots d\underline{r}_N$, $V(r_{ij})$ is the two-body potential energy and the ground state wave function Φ will be written in the form of equation (53),

$$\Phi = \prod_{i<j=1}{}' \left[1 + f(r_{ij})\right] .$$

This form for Φ was discussed in the last chapter. Also in the last chapter, Φ was written as a product of pair functions with no constraint,

$$\Phi = \prod_{i<j=1}^{N} \left[1 + f(r_{ij})\right] = \prod_{i<j=1}^{N} \psi(r_{ij}) \tag{77}$$

and the cluster integrals were introduced by first reducing the multi-dimensional integral in equation (1) to an integration over the relative distance between any pair of particles, say particles 1 and 2. This gives, for the expectation value of the energy per particle, equation (16)

$$\frac{\langle H \rangle}{N} = \frac{-\hbar^2}{2m}\int\left\{\left[\psi(r_{12})\nabla^2 \psi(r_{12})\right] C(r_{12}) + \frac{1}{2}\psi(r_{12})\nabla\psi(r_{12}) \cdot \nabla C(r_{12}) - \frac{m}{\hbar^2} V(r_{12}) \;{}^2(r_{12})\; C(r_{12})\right\} d\underline{r}_{12}$$

where the function $C(r_{12})$, defined by

$$C(r_{12}) = \frac{N(N-1)}{\rho^2 \psi^2(r_{12})} \frac{\int \prod_{i<j=1}^{N} \psi^2(r_{ij})\, d\underline{r}_3 \ldots d\underline{r}_N}{\int \prod_{i<j=1}^{N} \psi^2(r_{ij})\, d\underline{r}_1 \ldots d\underline{r}_N} \tag{78}$$

is related to the pair distribution function $n_2(r_{12})$ by

$$\rho^2 \psi^2(r_{12})\, C(r_{12}) = n_2(r_{12}) \; .$$

As indicated in Chapter II, the function $C(r_{12})$ can be expressed in a formal cluster expansion in powers of the density

$$C(r_{12}) = 1 + \sum_{n=1}^{\infty} \rho^n \xi_n (r_{12}) \qquad)79)$$

where $\xi_n(r_{12}) = \frac{1}{n!}\int \sum \Pi h(r_{ij})\, d\underline{r}_3 \ldots d\underline{r}_{n+2}$

$$h(r_{ij}) = \psi^2(r_{ij}) - 1 = 2f(r_{ij}) + f^2(r_{ij})$$

and the integrand $\sum \prod h(r_{ij})$ indicates the sum of all connected products for which each particle of the set n is connected to particles one and two by an independent path. Now the potential energy contribution to $\langle H \rangle$ is given by

$$\frac{\langle V\rangle}{N} = \frac{\rho}{2} \int V(r_{12})\ \psi^2(r_{12})\ C(r_{12})\ d\underline{r}_{12}\ . \qquad (80)$$

As the discussion of Chapter II indicates, the evaluation of the integrals in equation (79) corresponding to clusters of considerable numbers of particles becomes prohibitively difficult without the restriction of non-repeated indices on the ground state wave function. However, the non-repeated indices requirement on the wave function uniquely selects out of this original set of cluster integrals a simple subset of so-called ring integrals. To show this, first denote by $C_v(r_{12})$ the C function for the potential energy part of $\langle H\rangle$ modified by the hypothesis of non-repeated indices. Since $\psi(r_{ij}) = 1 + f(r_{ij})$ equation (80) can be written in the form

$$\frac{\langle V\rangle}{N} = \frac{\rho}{2} \int \Big\{ V(r_{12})\ C_{v1}(r_{12}) + 2V(r_{12})\ f(r_{12})\, C_{v2}(r_{12}) + V(r_{12})\ f^2(r_{12})\ C_{v3}(r_{12}) \Big\}\ d\underline{r}_{12} \qquad (81)$$

Examine first the formal cluster expansion of $C_{v1}(r_{12})$:

$$C_{v1}(r_{12}) = 1 + \sum_{n=1}^{\infty} \rho^n\ \xi_{n1}(r_{12}) \qquad (82)$$

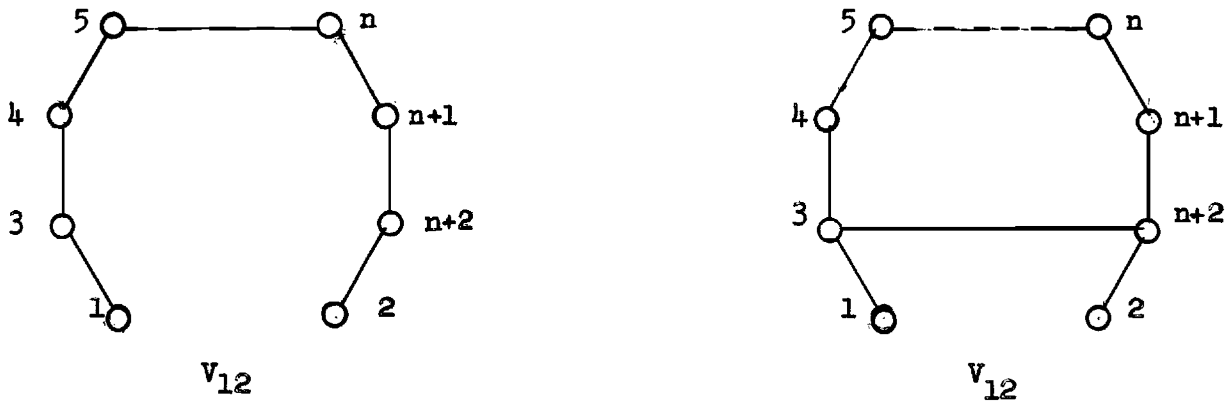
where

$$\xi_{n1}(r_{12}) = \frac{1}{n!} \int \sum_{(1)} \Pi h(r_{ij})\ d\underline{r}_3 \cdots d\underline{r}_{n+2} \qquad (83)$$

and the integrand $\sum_{(1)} \Pi h(r_{ij})$ indicates the sum of all connected products for which each particle of the set n is connected to particles one and two by an independent path and only those connected products are allowed which are consistent with the assumption of non-repeated indices in Φ. As a first consequence of the latter, only ring connected products are allowed. Those connected products with internal connections are not involved. For example a ring product such as illustrated in Figure is allowed, whereas a product with an internal connection (such as is illustrated in Figure 4(a) would imply the existence of repeated indices in Φ. Furthermore it should be noted that the $f^2(f_{ij})$ term in $h(r_{ij})$ is eliminated by the assumption of non-repeated indices. In the cluster expansion where repeated indices are allowed, the factor $2f(r_{ij})$ in equation (79) for $h(r_{ij})$ indicates that there are two places in any cluster from which each $f(r_{ij})$ may come, i.e., from Φ or Φ^*. In the case of non-repeated indices, this particular degeneracy is not present. For example, a ring of order $n = 3$ contains the product $f(r_{13})f(_{34})f(r_{45})$ $f(_{52})V(r_{12})$. The pair functions $f(r_{13})$ and $f(r_{45})$ may come from Φ while $f(r_{34})$ and $f(r_{52})$ must then come from Φ^*. Thus,

$$\xi_{n1}\,(r_{12}) = \frac{1}{n!} \int \sum \quad f(r_{ij})\; d\underline{r}_3 \ldots d\underline{r}_{n+2} \tag{84}$$

All the connected ring products illustrated in Figure 5 are allowed, but except for those in the first row they may be shown to contribute in the final result to a higher order. As a result, only those connected products illustrated in the first row of Figure 5 are included in the present calculation. All the connected products in Figure 5 are contained in the complete Hamiltonian for pair excitations which is treated in the next section. It should further be remembered that the connecting link between particles i and j in the connected products is now $f(r_{ij})$ and not the previous $2f(r_{ij}) + f^2(f_{ij})$.



a b

Figure 4. Certain Connected Products

(a) A typical ring connected product (b) A connected product which vanishes for non-repeated indices.

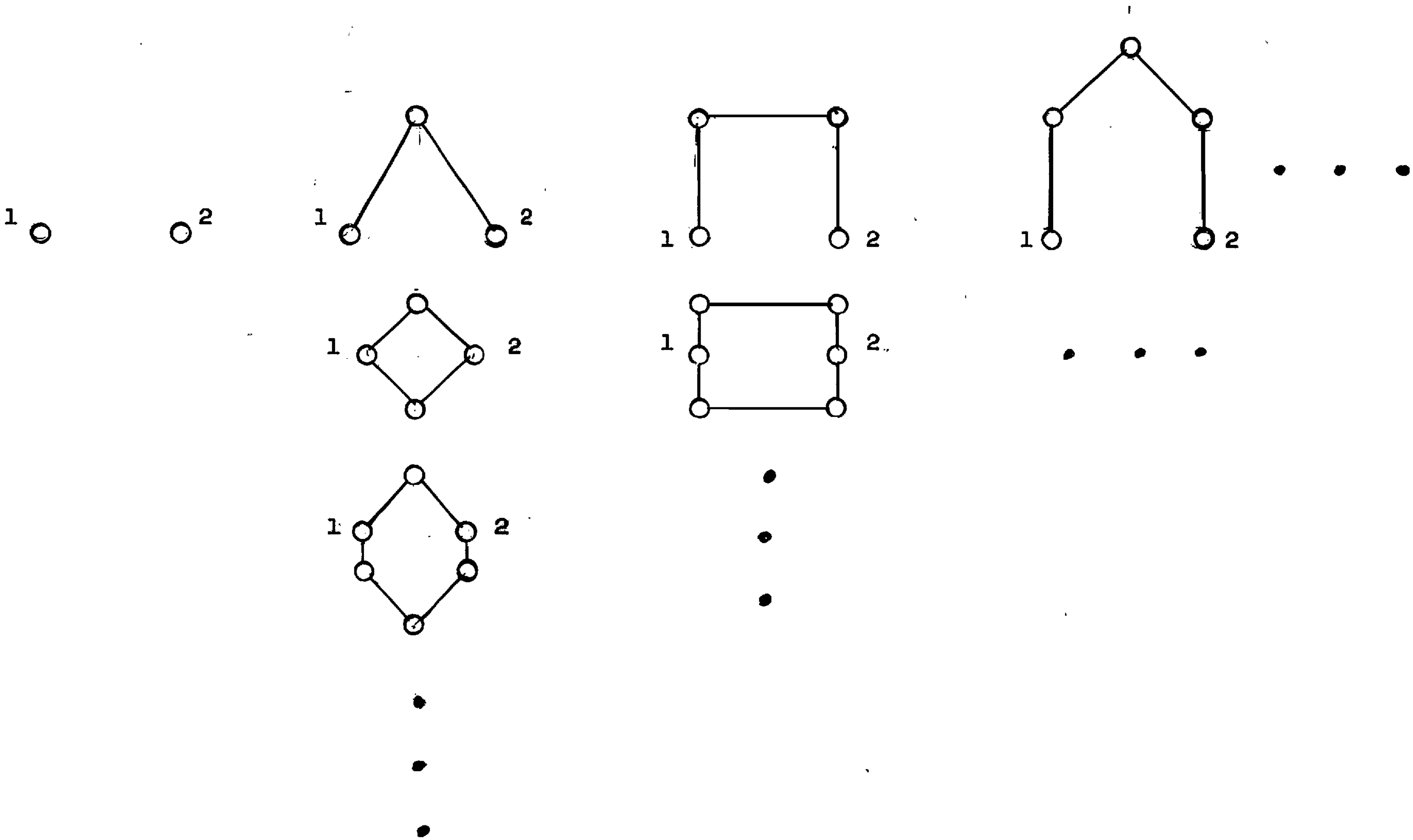


Figure 5. Graphs Representing the Contributions to $\langle V \rangle$ from the Terms $V(r_{12})\ C_{V_1}(r_{12})$

To evaluate $\xi_{n_1}(r_{12})$, note that permuting the n particles produces n! similar configurations, while there are also two ways of drawing the configuration from Φ and Φ^*. Hence

$$\sum \Pi f(r_{ij}) = 2(n!)\, f(r_{13})\, f(r_{34}) \ldots f(r_{n+1,n+2})\, f(r_{n+2,2}) \quad (85)$$

and

$$\xi_{n1}(r_{12}) = 2\int f(r_{13})\, f(r_{34}) \ldots f(r_{n+2,2})\, d\underline{r}_3 \ldots d\underline{r}_{n+2} \quad (86)$$

Introduce $\gamma(\underline{k})$, the Fourier transform of $f(\underline{r})$

$$\gamma(k) = \int f(\underline{r})\, e^{i\underline{k}\cdot\underline{r}}\, d\underline{r} \quad (87)$$

Then the function $\xi_{n1}(r_{12})$ becomes

$$\xi_{n1}(r_{12}) = \frac{2}{(2\pi)^3}\int \left[\gamma(k)\right]^{n+1} e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \quad (88)$$

and thus

$$C_{v1}(r_{12}) = 1 + \frac{2}{(2\pi)^3\rho}\sum_{n=1}^{\infty}\int \left[\rho\gamma(k)\right]^{n+1} e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \quad (89)$$

Interchanging the order of summation and integration, if $|\rho\gamma(k)| < 1$, one has

$$C_{v1}(r_{12}) = 1 + \frac{2\rho}{(2\pi)^3}\int \frac{\gamma^2(k)}{1-\rho\gamma(k)}\, e^{ik\cdot r_{12}}\, d\underline{k} \quad (90)$$

Next consider the second term in $\langle V\rangle/N$ given in equation (81), i.e.,

$$V(r_{12})\; 2f(r_{12})C_{v2}(r_{12}) \quad (91)$$

Note that C_{v2} may also be expanded in a cluster expansion,

$$C_{v2} = 1 + \sum_{n=1}^{\infty} \rho^n \, \xi_{n2} \, (r_{12}) \tag{92}$$

where

$$\xi_{n2}(r_{12}) = \frac{1}{n!} \int \sum_{(2)} \Pi f(r_{ij}) \, d\underline{r}_3 \ldots d\underline{r}_{n+2} \tag{93}$$

in accordance with the previous remarks in discussing the expansion of $C_{v1}(r_{12})$. As before, the integrand $\sum_{(2)} \Pi f(r_{ij})$ indicates the sum of all connected products for which each particle of the set n is connected to particles one and two by an independent path and only those connected products are allowed which are consistent with the assumption of non-repeated indices in Φ . In this case, terms of the form $V(r_{12})$ $(2f(r_{12}))\, \Pi f(r_{ij})$ are under consideration. Evaluation of $\sum_{(2)} \Pi f(r_{ij})$ will be made for the cases of n odd and even. Consider the example for n odd i.e., $\kappa = 3$, illustrated in Figure 6(a) . If $f(r_{12})$ came from Φ , then the hypotheses of non-repeated indices requires $f(r_{13})$ and $f(r_{52})$ to come from Φ^*. But this would imply that both $f(r_{34})$ and $f(r_{45})$ must come from Φ , which contradicts the assumption. Hence

$$\sum_{(2)} \Pi f(r_{ij}) = 0 \qquad \text{for n odd} \tag{94}$$

For those connected ring products for which n is even, terms of the type $V(r_{12})$ $2f(r_{12})$ $\Pi f(r_{ij})$ are to be examined under the hypothesis of non-repeated indices. Noting the example illustrated in Figure 6(b) , for $n = 4$, one observes that if $f(r_{12})$ came from Φ , then $f(r_{13})$ and $f(r_{62})$ must come from Φ^*, $f(r_{34})$, $f(r_{56})$ must come from Φ , and $f(r_{45})$ must come from Φ^*. Similarly one may have such a connected ring product if $f(r_{12})$

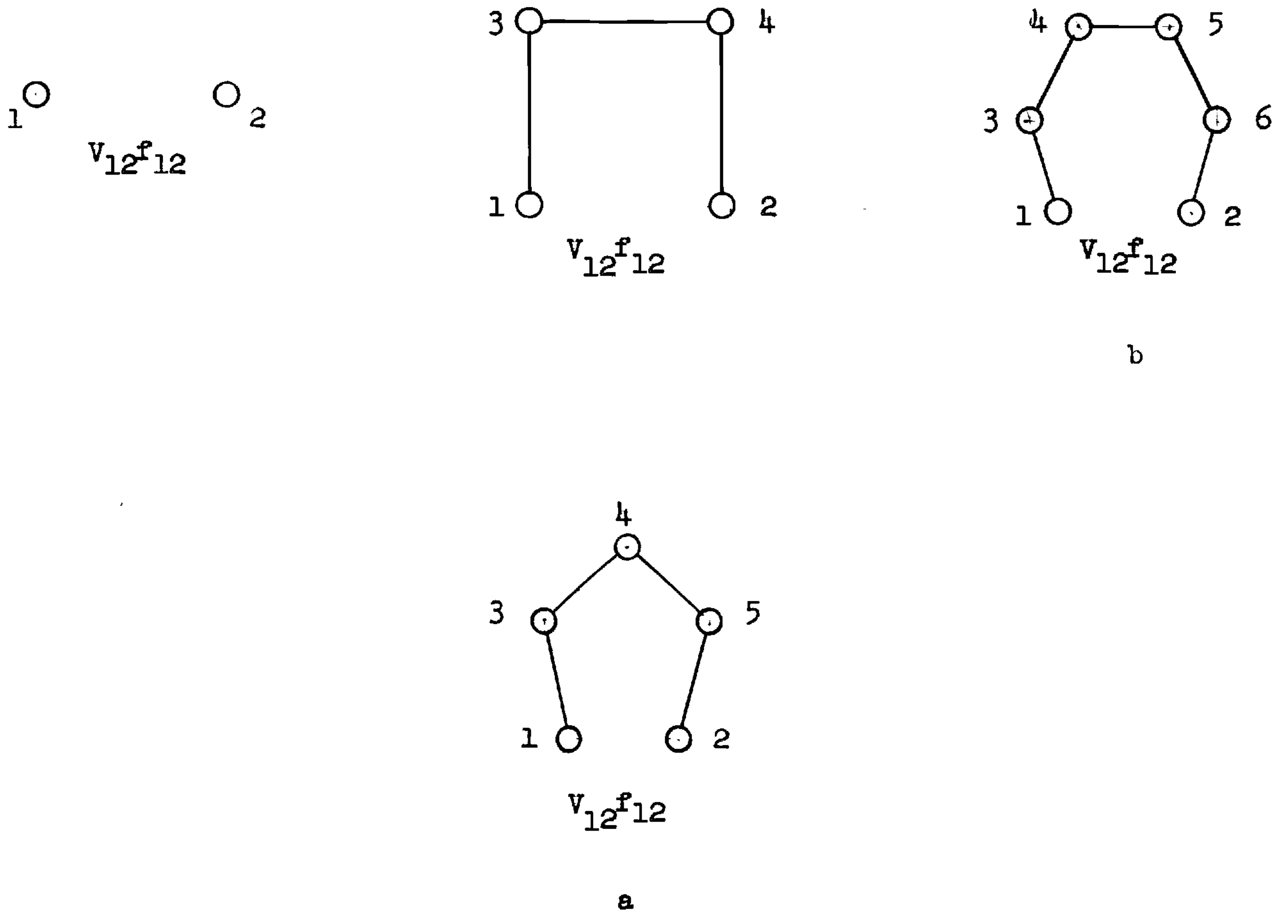


Figure 6. Graphs Representing the Successive Contributions to $\langle V \rangle$ from the term $V(r_{12})\ f(r_{12})\ Cv_1(r_{12})$. a) vanishes for non-repeated indices.

came from Φ^*. This is the significance of the factor two in the term

$$V(r_{12})\ \left[2f(r_{12})\right]\ \Pi f(r_{ij}),\ \text{i.e.}$$

there are two ways of drawing the configuration, from Φ and from Φ^*. In addition, permuting the n particles produces n! similar configurations. Hence

$$\sum_{(2)} \Pi f(r_{ij}) = n!\ f(r_{13})\ldots f(r_{n+2,2})\ \text{for n even} \tag{95}$$

This gives the result for $\xi_{n2}(r_{12})$,

$$\xi_{n2}(r_{12}) = \begin{cases} 0 & \text{n odd} \\ \dfrac{1}{(2\pi)^3}\displaystyle\int \left[\gamma(k)\right]^{h+1} e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} & \text{n even} \end{cases} \tag{96}$$

and, if $\left|\rho^2\,\gamma^2\,i(k)\right| < 1$,

$$C_{v2}(r_{12}) = 1 + \frac{\rho^2}{(2\pi)^3}\int \frac{\gamma^3(k)}{1-\rho^2\,\gamma^2(k)}\ e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \tag{97}$$

The last term in $\langle V\rangle/N$ is

$$V(r_{12})\ f^2(r_{12})\ C_{v3}(r_{12})\ . \tag{98}$$

The hypothesis of non-repeated indices requires that $C_{v3}(r_{12}) = 1$. This means that products which connect particles one and two are impossible, inasmuch as one $f(r_{12})$ in equation (98) must come from Φ and the other from Φ^*. In the present calculation, both this term and the second term in equation (97) are dropped, since they may both be shown to contribute to a higher order in the final result for the energy. Together with the diagrams in Figure 5 which were omitted earlier, they will be included in the calculations of the next section. Combining the above results yields the expectation value for the potential energy per particle as

$$\frac{\langle V \rangle}{N} = \frac{\rho}{2} \int V(r_{12}) \left\{ 1 + 2f(r_{12}) + \frac{2\rho}{(2\pi)^3} \int \frac{\gamma^2(k)}{1-\rho\gamma(k)} e^{i\underline{k}\cdot\underline{r}_{12}} d\underline{k} \right\} d\underline{r}_{12} \quad (99)$$

The first term in the integral on the right side of equation (99) represents the interaction between unexcited particles one and two and is shown graphically by the first term in the first row of Figure 5. The next term refers to the excitation and de-excitation of the pair (1,2) from and to the free particle ground state. The third and last term represents the sum of all contributions depicted by the remaining graphs shown in the first row of Figure 5, corresponding to multiple pair excitations and their interaction with the unexcited particles. The inclusion of only the integral obtained from the first term in the series for this sum, i.e., single pair excitations and their interaction with the ground state was made in the direct calculation, in the first section of this chapter. The diagrams contributing to equation (99) for $\langle V \rangle /N$ are shown in Figure 7.

Now for non-repeated indices the expectation value for the kinetic energy per particle is from equation (15),

$$\frac{\langle T \rangle}{N} = \frac{-\hbar^2}{2m} \int \psi(r_{12}) \nabla^2 \psi(r_{12})\; C_T(r_{12})\; d\underline{r}_{12}$$

$$= \frac{-\hbar^2}{2m} \int \left\{ \left[\nabla^2 f(r_{12})\right] C_{T1}(r_{12}) + \left[f(r_{12}) \nabla^2 f(r_{12})\right] C_{T2}(r_{12}) \right\} d\underline{r}_{12}$$

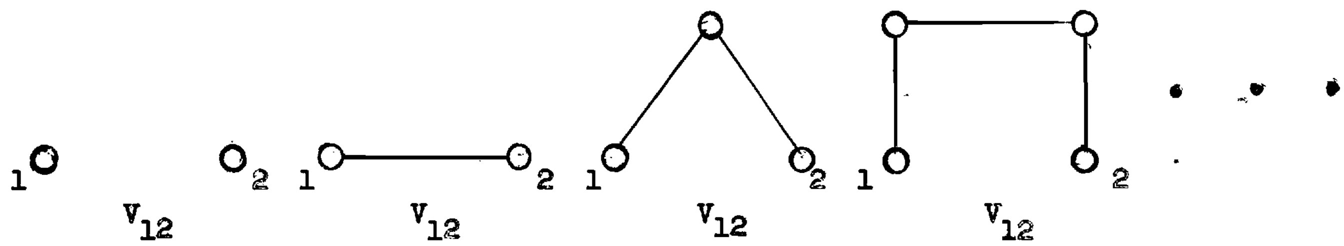


Figure 7. Cluster Diagrams Contributing to Equation (99) for $\langle V \rangle/N$

It is important to notice the absence of a term $\nabla f \cdot \nabla C$. Such a term arises from products such as $\nabla_1^2 \left[f(r_{12})\ f(r_{13})\ f(r_{45})\right]$

$$\nabla_1 \cdot \left[f(r_{13})\ f(r_{45}) \nabla_1 f(r_{12}) + f(r_{12})\ f(r_{45})\ \nabla_1 f(r_{13})\right] \tag{100}$$

$$= \left[\nabla_1^2\ f(r_{12})\right]\ f(r_{13})\ f(r_{45}) + f(r_{12})\ f(r_{45}) \nabla_1^2 f(r_{13})$$
$$+ 2f(r_{45}) \nabla_1 f(r_{12}) \cdot \nabla_1 f\ (r_{13})\ .$$

But such products are missing in Φ , due to non-repeated indices.

In a similar manner to the treatment of $\langle V \rangle / N$, a cluster expansion may be made of $C_{Ti}(r_{12})$ of the form

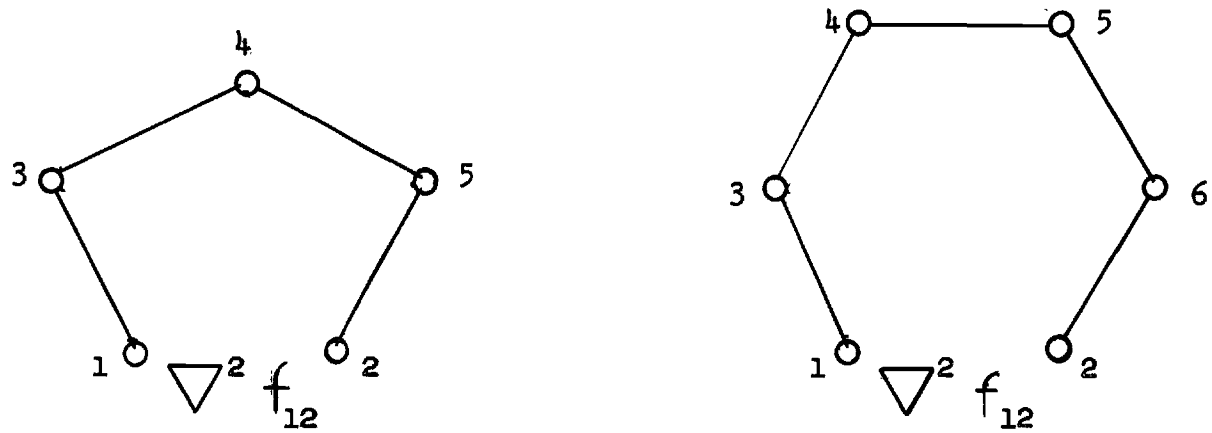
$$C_{Ti}\ (r_{12}) = 1 + \sum_{n=1} \rho^n\ \xi_{ni}(r_{12}) \quad i = 1,2 \tag{101}$$

where

$$\xi_{ni}\ (r_{12}) = \frac{1}{n!} \sum_{(T_i)} \Pi f(r_{ij})\ d\underline{r}_3 \ldots d\underline{r}_{n+2} \tag{102}$$

Consider $\sum_{(T1)} \Pi f(r_{ij})$, and do so first for those connected products for which n is odd. The example n = 3 is shown in Figure 8 . For C_{T1} terms of the form $\nabla^2 f(r_{12})\ \ \Pi f(r_{ij})$ are involved. Since $f(r_{12})$ comes from Φ, then $f(r_{13})$ and $f(r_{52})$ in the illustrated example, must come from Φ^*. Thus $f(r_{34})$ and $f(r_{45}$ must come from Φ.which contradicts the assumption of non-repeated indices. In general, the conclusion is that

$$\sum_{(T1)} \Pi f(r_{ij}) = 0 \quad \text{for n odd.} \tag{103}$$



a b

Figure 8. Graphs Representing Contributions to the Kinetic Energy from the term $\nabla^2 f(r_{12})\ C_{r_1}(r_{12})$. (a) A term with odd n, (n = 3) which vanishes for the non-repeated indices. (b) A term with even n (n=4) which gives a non-vanishing contribution.

Next $\sum_{(T1)} \Pi f(r_{ij})$ is examined for those connected products for which n is even. The example n = 4 is shown in Figure 8(b). This example is the term $\nabla^2 f(r_{12}) \left[f(r_{13})\ f(r_{34})\ f(r_{45})\ f(r_{56})\ f(r_{62})\right]$. Since $f(r_{12})$ comes from Φ, then $f(r_{13})$ and $f(r_{62})$ must come from Φ^*, $f(r_{34})$ and $f(r_{56})$ must come from Φ, and $f(r_{45})$ must come from Φ^*, all required by the hypothesis of non-repeated indices. There is only one way of drawing the configuration for $\nabla^2 f(r_{12})\ \Pi f(r_{ij})$ from Φ and Φ^* since $f(r_{12})$ must come from Φ. Permuting the n particles does produce n! similar configurations. The general conclusion is

$$\sum_{(T_1)} \Pi f(r_{ij}) = n!\ f(r_{13})\ f(r_{34})\ \ldots\ f(r_{n+2,2}) \text{ for n even.} \tag{104}$$

This gives the result for the function

$$\xi_{n1}(r_{12}) = \frac{1}{h!} \int \sum_{(T_1)} \Pi f(r_{ij})\ d\underline{r}_3 \ldots d\underline{r}_{n+2} \tag{105}$$

as

$$\xi_{n1}(r_{12}) = \begin{cases} 0 & ,\ \text{n odd} \\ \dfrac{1}{(2\ )^3} \displaystyle\int \left[\gamma(k)\right]^{h+1} e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k}, & \text{n even} \end{cases} \tag{106}$$

Performing the sum over n, after interchanging the order of integration and summation, leads to the result

$$C_{T1}(r_{12}) = 1 + \frac{\rho^2}{(2\pi)^3} \int \frac{\gamma^3(k)}{1-\rho^2\gamma^2(k)}\ e^{i\underline{k}\cdot\underline{r}_{12}}\ d\underline{k}, \tag{107}$$

if $|\rho^2\gamma^2| < 1$.

Now consider $\sum_{(T_2)} \Pi f(r_{ij})$. In this case terms of the form $f(r_{12}) \nabla^2 f(r_{12}) \; \Pi f(r_{ij})$ are involved. As the assumption of non-repeated indices requires one $f(r_{12})$ to come from Φ while the other must come from Φ^*, it also implies there are no additional connections in the product. Hence

$$\sum_{(T_2)} \Pi f(r_{ij}) = 0 \quad \text{and} \quad C_{T_2}(r_{12}) = 1 \, . \tag{108}$$

With the results of equation (107) for $C_{T1}(r_{12})$ and equation (108) for $C_{T2}(r_{12})$, the expectation value for the kinetic energy may finally be written as

$$\frac{\langle T\rangle}{N} = \frac{-\rho\hbar^2}{2m} \int \nabla^2 f(r_{12}) \Bigg\{ 1 + f(r_{12}) + \frac{\rho^2}{(2\pi)^3} \int \frac{\gamma^3(k)}{1-\rho^2 \gamma^2(k)} \; e^{i\underline{k}\cdot\underline{r}_{12}} \, d\underline{k} \Bigg\} d\underline{r}_{12} \tag{109}$$

The expectation value for the energy per particle in the present approximation is then obtained by adding equation (99) and equation (109).

To make connection with the results from the perturbation theory calculation for hard spheres, the pseudopotential shown by Lee, Huang, and Yang (36) to be applicable to this interaction at the low densities considered here is now used for V(r). As pointed out in the last chapter, they have shown that it is essential, in order to remove spurious infinities, to use the correct pseudopotential,

$$V(r) = g \, \delta(\underline{r}) \, \frac{\partial}{\partial r} \, (r \quad , \quad g = \frac{4\pi a\hbar^2}{m} \tag{110}$$

where a is the hard sphere diameter. Actually, one can use the form $V(r) = g\,\delta(\underline{r})$, and switch to the correct form given in equation (110) at the end of the calculation. In addition, the expression for $\langle H \rangle$ is considerably simplified by transforming the pair function $f(r_{12})$ to momentum space. As shown in Appendix B, the result is

$$\frac{\langle H\rangle}{N} = \frac{\hbar^2}{2m}\left\{\frac{g_1}{2} + \frac{1}{(2\pi)^3}\int \frac{k^2\gamma^2 + g_1\gamma + \rho g_1\gamma^2}{1-\rho^2\gamma^2}\, d\underline{k}\right. \tag{111}$$

where $g_1 = 8\pi a$. Varying $\langle H\rangle/N$ with respect to $\gamma(k)$ yields the Euler equation:

$$\frac{g_1\rho^2\gamma^2 + 2(g_1\rho + \gamma k^2) + g_1}{(1-\rho^2\gamma^2)^2} = 0 \tag{112}$$

Its solution for $\gamma(k)$ is

$$\rho\gamma(k) = -\left(1 + \frac{k^2}{\rho g_1}\right) + \frac{k}{\rho g_1}\sqrt{k^2 + 2\rho g_1} \tag{113}$$

where the + sign is chosen in front of the radical to satisfy the condition that $|\rho\gamma(k)| < 1$. Substituting for $\gamma(k)$ in equation (111) one obtains

$$\frac{\langle H\rangle}{N} = \frac{2\pi a\hbar^2\rho}{m}\left[1 + \lim_{r\to o}\frac{\partial}{\partial r}\, r\int \gamma(k)\, e^{i\underline{k}\cdot\underline{r}}\, d\underline{k}\right] \tag{114}$$

Evaluating the integral yields the result

$$E_o = \langle H\rangle = \frac{2\pi N\rho a\hbar^2}{m}\left[1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{\frac{1}{2}}\right] \tag{115}$$

which is the result previously obtained from perturbation theory (37), (38). Using the solution for $\gamma(k)$ from equation (113), the neglected terms in the development for the potential energy are easily shown to contribute to the energy in the order $\rho^2 a^4$, and hence in a higher approximation. Calculations of other ground state characteristics such as the depletion factor are also in agreement.

Complete Multiple Pair Excitations.--In order to calculate the complete ground state Hamiltonian for pair excitations using the wave function in configuration space

$$\Phi = \Pi' \,(1 + f(r_{ij})) \tag{116}$$

and the cluster expansion approach, those diagrams which are consistent with this wave function and were omitted from the expectation value of the potential energy per particle, $\langle V \rangle /N$, in the cluster expansions of the last section must now be calculated and their contributions included. Those diagrams which were included in the last section are shown in Figure 7 and their contribution to $\langle V \rangle /N$ is given by equation (99). The omitted diagrams will be discussed and their contribution will be calculated in this section. The expectation value of the kinetic energy per particle, $\langle T \rangle /N$ was calculated for the wave function of equation (116) in the last section, using cluster expansions. From equation (110)

$$\frac{\langle T \rangle}{N} \quad \frac{-\rho h^2}{2m} \int \nabla^2 f(r_{12}) \left\{ 1 + f(r_{12}) + \frac{\rho^2}{(2\pi)^3} \int \frac{\gamma^3(k)}{1 - \rho^2 \gamma^2(k)} \, e^{i\underline{k}\cdot\underline{r}_{12}} \, d\underline{k} \right\} d\underline{r}_{12} \tag{117}$$

or, with $f(r_{12})$ transformed to momentum space by

$$f(r_{12}) = \frac{1}{(2\pi)^3} \int \gamma(k)^{i\underline{k}\cdot\underline{r}_{12}} \, d\underline{k} \tag{118}$$

one has, from Appendix B, equations (216)-(218) that

$$\frac{\langle T\rangle}{N} = \frac{\rho h^2}{2m}\ \frac{1}{(2\pi)^3}\int\left(k^2\gamma^{\,2} + \frac{\gamma^2\rho k^2\ \gamma^4}{1-\rho^2\gamma^2}\right)\,d\underline{k} \tag{119}$$

$$= \frac{\rho h^2}{2m}\ \frac{1}{(2\pi)^3}\int\frac{k^2\ \gamma^2}{1-\rho^2\gamma^2}\quad d\underline{k}\ .$$

Indicating by $\left[\frac{\langle V\rangle}{N}\right]_1$, that part of $\frac{\langle V\rangle}{N}$, determined by those diagrams in the cluster expansions which were counted in the last section, one has from equation (99)

$$\left[\frac{\langle V\rangle}{N}\right]_1 = \frac{\rho}{2}\int\Bigg\{V(r_{12}) + 2V(r_{12})\ f(r_{12})$$

$$+ \frac{2V(r_{12})}{(2\pi)^3}\int\frac{\rho^2}{1-\rho\gamma}\quad e^{i\underline{k}\cdot\underline{r}_{12}}\ d\underline{k}\Bigg\}\,d\underline{r}_{12}$$

With $f(r_{12})$ transformed to momentum space by equation (118) and $V(r_{12})$ transformed by

$$V(r_{12}) = \frac{1}{(2\pi)^3}\int v(k)\ e^{i\underline{k}\cdot\underline{r}_{12}}\ d\underline{k} \tag{120}$$

this expression is considerably simplified. As shown in Appendix C, the result is

$$\left[\frac{\langle V\rangle}{N}\right]_1 = \frac{\rho v(o)}{2} + \frac{1}{(2\pi)^3}\int\Bigg\{\rho v(k)\ \gamma(k) \tag{121}$$

$$+ \frac{\rho^2\ v(k)\ \gamma^2(k)}{1-\rho\gamma(k)}\Bigg\}\,d\underline{k}$$

$$= \frac{\rho v(o)}{2} + \frac{1}{(2\pi)^3}\int\rho\, v(k)\ \frac{\gamma(k)}{1-\rho\gamma(k)}\quad d\underline{k}$$

The part of $\frac{\langle V\rangle}{N}$ which is determined by those diagrams which were omitted in the last section will be designated by $\left[\frac{\langle V\rangle}{N}\right]_2$. These diagrams correspond to interactions between excited pairs. They arise from the cluster expansions of the functions $C_{v_1}(r_{12})$, $C_{v_2}(r_{12})$ and $C_{v_3}(r_{12})$ in equation (81). To calculate the contribution of the previously omitted diagrams, the cluster expansions of the C_v functions will now be examined. Consider first the term in $\frac{\langle V \rangle}{N}$ involving $C_{v_3}(r_{12})$,

$$\int V(r_{12})\, f^2(r_{12})\, C_{v_3}(r_{12})\, d\underline{r}_{12} \,. \tag{122}$$

From the discussion of equation (98), C_{v_3} 1. Hence equation (122), after $f(r_{12})$ and $V(r_{12})$ have been transformed to momentum space in accordance with equation (118) and equation (120)

$$\int V(r_{12})\, f^2(r_{12})\, d\underline{r}_{12} = \int V(r_{12}) \left[\frac{1}{(2\pi)^3} \int \gamma(k)\, e^{-i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k}\right] \cdot \left[\frac{1}{(2\pi)^3} \int \gamma(k')\, e^{i\underline{k}'\cdot\underline{r}_{12}}\, d\underline{k}'\right] d\underline{r}_{12}$$

$$= \frac{1}{(2\pi)^6} \int \left[v(k-k')\ \gamma(k')\ \gamma(k)\right] d\underline{k}'\, d\underline{k}$$

For the purposes of the eventual summation, this contribution is entered diagrammetrically in the first row and first column of Figure 9 . Next, consider the term in $\frac{\langle V \rangle}{N}$ involving $C_{v_2}(r_{12})$, i.e.

$$\int V(r_{12}) \left[2f(r_{12})\right] C_{v_2}(r_{12})\, d\underline{r}_{12} \,. \tag{123}$$

As determined in the last section, one has from equation (97) for the cluster expansion of $C_{v_2}(r_{12})$,

$$C_{v_2}(r_{12}) = 1 + \frac{\rho^2}{(2\pi)^3} \int \frac{\gamma^3(k)}{1 - \rho^2\, \gamma^2(k)}\, e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k},\ \left|\rho^2\, \gamma^2(k)\right| < 1$$

With this expression for $C_{v_2}(r_{12})$, equation (123) becomes

$$\int V(r_{12}) \left[2f(r_{12})\right] C_{v_2}(r_{12})\, d\underline{r}_{12} \tag{124}$$

$$= \int 2V(r_{12}) f(r_{12}) + V(r_{12}) \quad \frac{2f(r_{12})\ \rho^2}{(2\ )^3} \int \frac{\gamma^3(k)}{1 - \rho^2 \gamma^2(k)}\, e^{i\underline{k}\cdot\underline{r}_{12}} d\underline{k}\ \ d\underline{r}_{12}$$

The first term in the integral on the right was included in the last section and hence in $\left[\frac{\langle V\rangle}{N}\right]_1$, equation (99). The remainder of this integral, after transformation of $f(r_{12})$ and $V(r_{12})$ to momentum space, is

$$\frac{2}{(2\pi)^6} \int \left\{ v(k-k')\ \gamma(k')\ \frac{\left[\rho^2\ \gamma^3\ (k)\right]}{1 - \rho^2\ \gamma^2(k)} \right\} d\underline{k}' d\underline{k}$$

or, since $v(\underline{k}) = v(-\underline{k})$

$$\frac{1}{(2\pi)^6} \int \Bigg\{ v(k-k')\ \gamma(k')\ \gamma(k) \sum_{n=1} \left[\rho^2\ \gamma^2(k)\right]^n$$

$$+\ v(k-k')\ \gamma(k') \sum_{n=1}^{\infty} \left[\rho^2\ \gamma^2(k')\right]^n \cdot \gamma\ (k) \Bigg\}\ d\underline{k}' d\underline{k}$$

In the above, the geometric sum was reexpanded and k and k' relabeled, for the group of terms. Diagrammatically, these terms are entered in the remaining places of the first row and first column of Figure 9 .

The term involving $C_{v_1}(r_{12})$ in $\frac{\langle V\rangle}{N}$ is

$$\int V(r_{12})\ C_{v_1}\ (r_{12})\ d\underline{r}_{12} \tag{125}$$

From the cluster expansion of $C_{v_1}(r_{12})$, only those terms depicted in the first row of Figure 5 were included in $\left[\frac{V}{N}\right]_1$. The remaining terms to be examined are shown in the other rows of this figure. They are connected products for which each particle of the set n is connected to

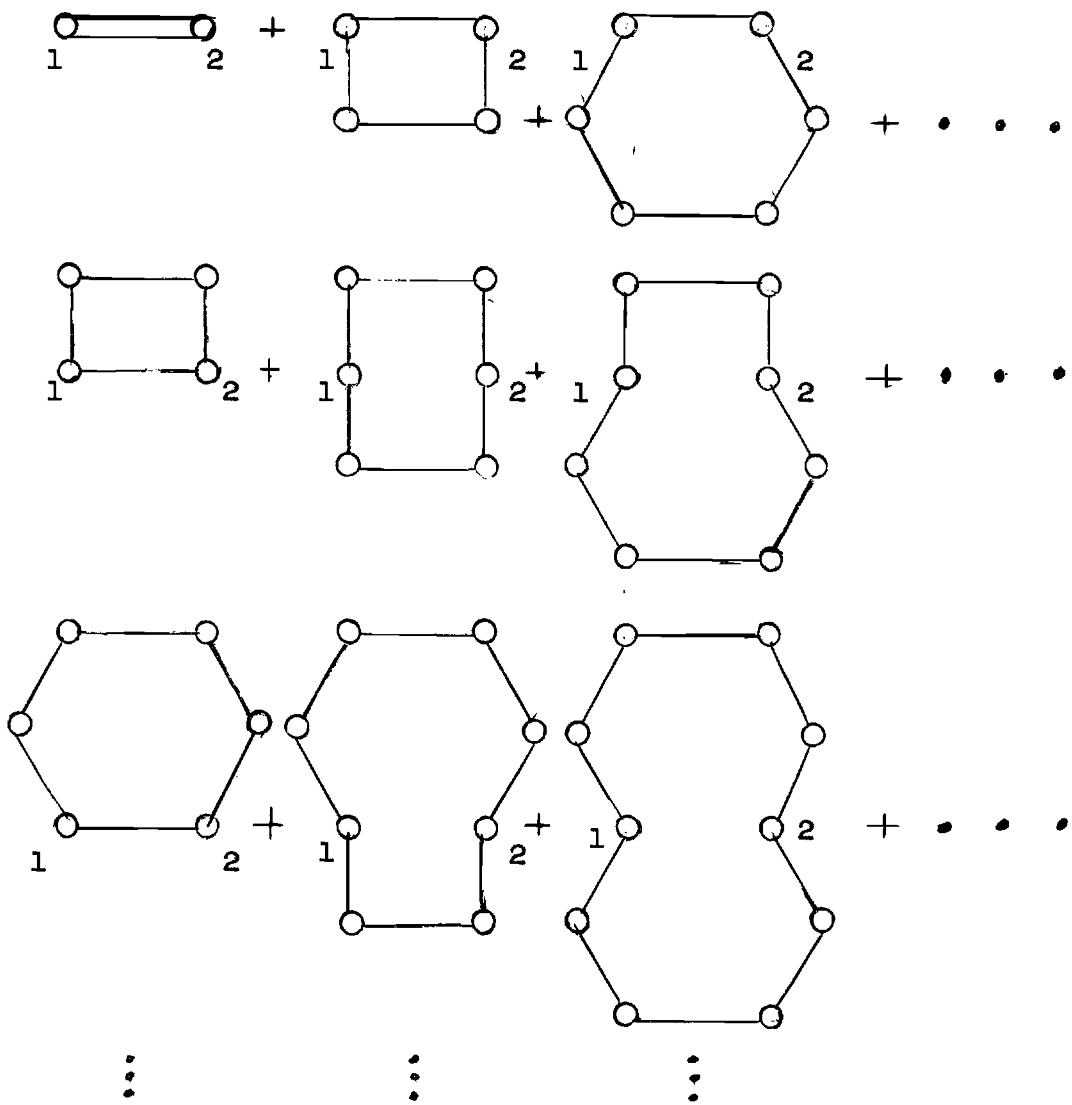


Figure 9. Cluster Diagrams Included in Equation (143)

particles one and two by an independent path. This is in accordance with the defining prescription, which accompanied equation (79). These connected products are of the "separable" type. The meaning of this will soon become clear. Consider now several typical ones of the connected products involved. First, for n = 2

$$\frac{1}{2!}\int\sum f(r_{13})\ f(r_{32})\ f(r_{14})\ f(r_{42})\ d\underline{r}_3 d\underline{r}_4\ . \tag{126}$$

Permuting the two particles does not produce a new configuration, but there are two ways of drawing the configuration from Φ and Φ^*. Thus, equation (126) becomes

$$\frac{2}{2!}\int f(r_{13})\ f(r_{32})\ f(r_{14})\ f(r_{42})\ d\underline{r}_3 d\underline{r}_4 . \tag{127}$$

But the integral involved separates, so that one has

$$\left[\int f(r_{13})\ f(r_{32})\ d\underline{r}_3\right]\ \left[\int f(r_{14})\ f(r_{42}) d\underline{r}_4\right] \tag{128}$$

The connected product is thus separated into the product of the connected product for the particle above an imaginary line joining particles one and two and the connected product for the particle below.

For n = 3, the hypothesis of non-repeated indices eliminates a connected product such as illustrated in Figure 10(a). In general, there will be no connected products with an even number of particles above the imaginary line and an odd number below it or vice-versa. This means that for n odd, there are no separable connected products. For n = 4, there are two different types of the connected products remaining to be counted.

First, as illustrated in Figure 10(b), there is

$$\frac{1}{4!}\int\sum f(r_{13})\ f(r_{34})\ f(r_{42})\ f(r_{26})\ f(r_{65})\ f(r_{51})d\underline{r}_3 d\underline{r}_4 d\underline{r}_5 d\underline{r}_6 \quad (129)$$

Permuting the four particles produces twelve new configurations. There are also two ways of drawing the configuration from Φ and Φ^*. As a result, equation (129) becomes

$$\frac{12.2}{4!}\int f(r_{13})\ f(r_{34})\ f(r_{42})\ f(r_{26})\ f(r_{65})\ f(r_{51})\ d\underline{r}_3 d\underline{r}_4 d\underline{r}_5 d\underline{r}_6 \quad (130)$$

This connected product separates into the product of the connected products for the two upper particles and the two lower ones, i.e.

$$\left[\int f(r_{13})\ f(r_{34})\ f(r_{42})\ d\underline{r}_3 d\underline{r}_4\right]\left[\int f(r_{15})\ f(r_{56})\ f(r_{62}) d\underline{r}_5 d\underline{r}_6\right] \quad (131)$$

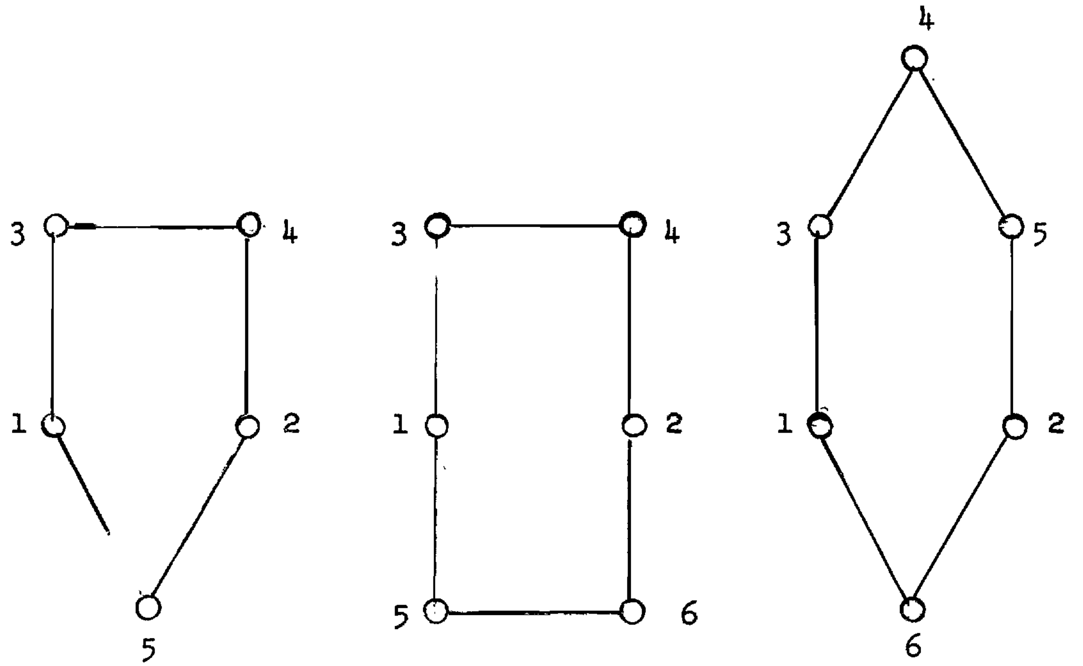
The remaining type of connected product for $n = 4$ is illustrated in Figure 10(c). This product is

$$\frac{1}{4!}\int\sum f(r_{13})\ f(r_{34})\ f(r_{45})\ f(r_{52})\ f(r_{26})\ f(r_{61})d\underline{r}_3 d\underline{r}_4 d\underline{r}_5 d\underline{r}_6 \quad (132)$$

In this case, permuting the $n = 4$ particles produces $n! = 4!$ new configurations. This is in contrast with the previous one where there was an equal number of particles both above and below the imaginary line. There are still two ways of drawing the configuration from Φ and Φ^*. In view of this, equation (132) becomes

$$\frac{4!2}{4!}\int f(r_{13})\ f(r_{34})\ f(r_{45})\ f(r_{52})\ f(r_{26})\ f(r_{61})d\underline{r}_3 d\underline{r}_4 d\underline{r}_5 d\underline{r}_6 \quad (133)$$

or when separated



a b c

Figure 10. Certain Cluster Diagrams

(a) Vanishes for Non-Repeated Indices, while (b) and (c) do not.

$$2\left[\int f(r_{13})\ f(r_{34})\ f(r_{45})\ f(r_{52})d\underline{r}_3 d\underline{r}_4 d\underline{r}_5\right]\left[\int f(r_{16})\ f(r_{62})d\underline{r}_6\right] \tag{134}$$

It thus separates into the product of the connected products for three particles above the line and one below, or vice-versa.

Of course, the integrals into which the connected products separate are of the faltung type discussed previously and hence, in terms of the transform $\gamma(k)$ of $f(r)$ a typical one becomes

$$\int f(r_{13})\ f(r_{34})\ f(r_{45})\ f(r_{52})d\underline{r}_3 d\underline{r}_4 d\underline{r}_5 = \frac{1}{(2\pi)^3}\int\left[\gamma(k)\right]^4 e^{i\underline{k}\cdot\underline{r}}\,d\underline{k}$$

The contribution of the connected product illustrated in Figure 10(c) and separated in equation (131) to $\frac{\langle V\rangle}{N}$ is

$$\int V(r_{12})\ \frac{\rho^4}{(2\pi)^6}\left\{\int\left[\gamma(k)\right]^3 e^{-i\underline{k}\cdot\underline{r}_{12}}\,d\underline{k}\right\}\left\{\int\left[\gamma(k')\right]^3 e^{i\underline{k}'\cdot\underline{r}_{12}}d\underline{k}'\right\}d\underline{r}_{12} \tag{135}$$

or

$$\frac{\rho^4}{(2\pi)^6}\int\left\{\nu(k-k')\ \gamma^3(k)\,\gamma^3(k')\right\}d\underline{k}'d\underline{k} \tag{136}$$

Those connected products with an equal number of particles above and below the imaginary line joining particles one and two are entered along the diagonals in Figures 9 and 11. In particular, those connected products with an even number above the line and an equal even number below are entered in Figure 9, while those with an odd number above and an equal odd number below the line are entered in Figure 11. Those connected products with an unequal number of particles above and below the imaginary line are entered in the off-diagonal places in the diagrams of Figure 9 and Figure 11. Since these connected products have a weight of two as

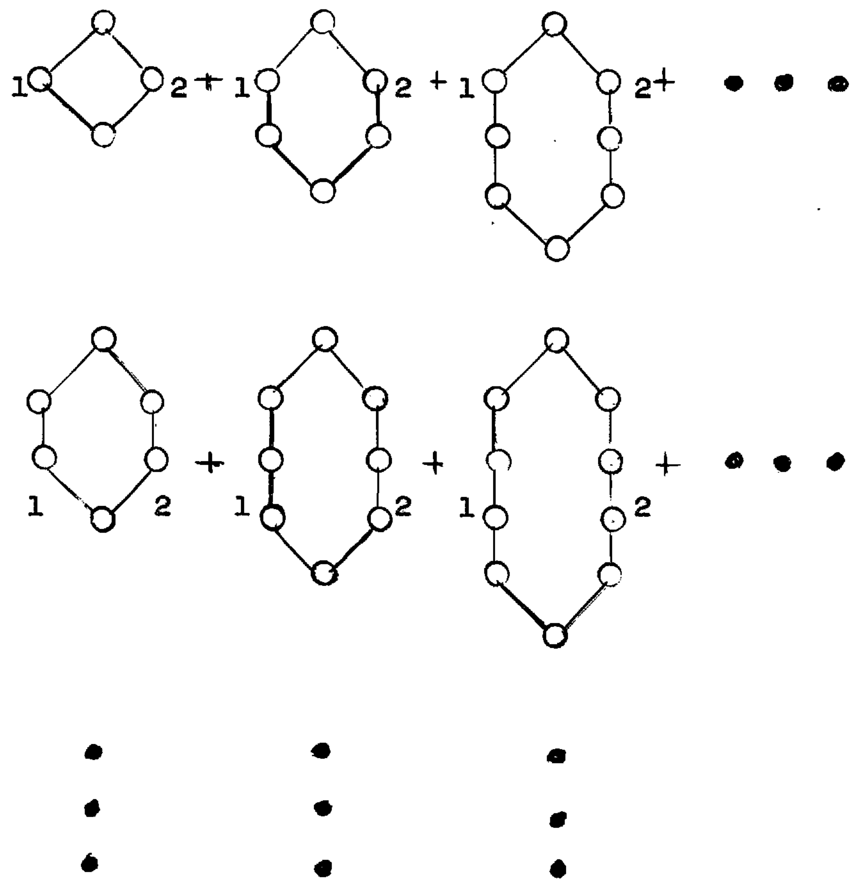


Figure 11. Cluster Diagrams Included in Equation (147)

compared with those on the diagonal, they will be entered with a weight of one in both the ij^{th} position and the symmetric ji^{th} position. If a connected product has an odd number of particles both above and below the imaginary line joining particles one and two, the numbers being unequal, it is entered in the appropriate off-diagonal positions in Figure 11. If it has an even number of particles both above and below the imaginary line, the numbers being unequal, the connected product is entered in the appropriate off-diagonal positions in Figure 9 . By this procedure, all those connected products which are consistent with the hypothesis of non-repeated indices and were omitted in the last section are depicted with equal weight in either Figure 9 or Figure 11.

With the aid of these diagrams, the contribution of those connected products may be summed. First consider Figure 9. Summing formally the contribution of the elements of the first row to $\langle V \rangle /N$ and transforming to momentum space, one has

$$\frac{\rho}{2}\int\left\{V(r_{12})\; f(r_{12})\left[f(r_{12})+\sum_{n=2,4,\ldots}^{\infty}\rho^{n}\int f(r_{13})\ldots f(r_{n+2,2})\cdot d\underline{r}_3\ldots d\underline{r}_{n+2}\right]\right\}d\underline{r}_{12} \tag{137}$$

$$=\frac{1}{(2\pi)^6}\;\frac{\rho}{2}\int v(k-k')\,\gamma(k)\left\{\gamma(k')+\frac{1}{\rho}\sum_{n=2,4,\ldots}^{\infty}\left[\rho\,\gamma(k')\right]^{n+1}\right\}d\underline{k}'d\underline{k}$$

$$=\frac{1}{(2\pi)^6}\;\frac{\rho}{2}\int v(k-k')\,\gamma(k)\;\frac{\gamma(k')}{1-\rho^2\,\gamma^2(k')}\;d\underline{k}'d\underline{k}$$

Summing formally the second row of Figure 9 , one has

$$\frac{1}{(2\pi)^6} \quad \frac{\rho}{2} \int v(\mathrm{k}-\mathrm{k}')\rho^2\gamma^3(\mathrm{k}) \quad \frac{\gamma(\mathrm{k}')}{1-\rho^2\gamma^2(\mathrm{k}')} \quad d\underline{\mathrm{k}}'d\underline{\mathrm{k}} \tag{138}$$

Similarly, the remaining rows when summed yield respectively,

$$\frac{1}{(2\pi)^6} \quad \frac{\rho}{2} \int v(\mathrm{k}-\mathrm{k}')\,\rho^4\gamma^5(\mathrm{k}) \frac{\gamma(\mathrm{k}')}{1-\rho^2\gamma^2(\mathrm{k}')} \quad d\underline{\mathrm{k}}'d\underline{\mathrm{k}} \tag{139}$$

$$\frac{1}{(2\pi)^6} \quad \frac{\rho}{2} \int v(\mathrm{k}-\mathrm{k}')\,\rho^6\gamma^7(\mathrm{k}) \quad \frac{\gamma(\mathrm{k}')}{1-\rho^2\gamma^2(\mathrm{k}')} \quad d\underline{\mathrm{k}}'d\underline{\mathrm{k}} \tag{140}$$

$$\frac{1}{(2\pi)^6} \quad \frac{\rho}{2} \int v(\mathrm{k}-\mathrm{k}')\,\rho^8\gamma^9(\mathrm{k}) \quad \frac{\gamma(\mathrm{k})}{1-\rho^2\gamma^2(\mathrm{k}')} \quad d\underline{\mathrm{k}}'d\underline{\mathrm{k}} \tag{141}$$

etc.

Now, summing formally the contributions of the rows, i.e., adding equations (137), (138), (139), (140), (141), etc. yields

$$= \frac{1}{(2\pi)^6} \quad \frac{\rho}{2} \int v(\mathrm{k}-\mathrm{k}')\left\{ \gamma(\mathrm{k}) + \rho^2\gamma^3(\mathrm{k}) + \rho^4\gamma^5(\mathrm{k}) + \ldots\right\} \frac{\gamma(\mathrm{k}')}{1-\rho^2\gamma^2(\mathrm{k}')} \quad d\underline{\mathrm{k}}'d\underline{\mathrm{k}} \tag{142}$$

$$= \frac{1}{(2\pi)^6} \quad \frac{\rho}{2} \int v(\mathrm{k}-\mathrm{k}') \frac{\gamma(\mathrm{k})}{1-\rho^2\gamma^2(\mathrm{k})} \quad \frac{\gamma(\mathrm{k}')}{1-\rho^2\gamma^2(\mathrm{k}')} \, d\underline{\mathrm{k}}'d\underline{\mathrm{k}}$$

Thus the contribution of the terms depicted in Figure 9 to $\frac{\langle V\rangle}{N}$ is

$$\frac{1}{(2\pi)^3} \quad \frac{\rho}{2} \int\left\{\frac{1}{(2\pi)^3}\right\} v(\mathrm{k}-\mathrm{k}') \frac{\gamma(\mathrm{k}')}{1-\rho^2\gamma^2(\mathrm{k}')} \quad d\underline{\mathrm{k}}'\Big\} \frac{\gamma(\mathrm{k})}{1-\rho^2\gamma^2(\mathrm{k})} \, d\underline{\mathrm{k}} \tag{143}$$

A similar procedure may be applied to summing the contributions of the diagrams in Figure 11. Formally summing the first row gives

$$\frac{\rho}{2}\frac{1}{(2\pi)^6}\int v(\mathbf{k}-\mathbf{k}')\rho\gamma^2(\mathbf{k})\left\{\rho\gamma^2(\mathbf{k}')+\rho^3\gamma^4(\mathbf{k}')+\rho^5\gamma^6(\mathbf{k}')+\ldots\right\}d\underline{k}'d\underline{k} \tag{144}$$

$$=\frac{1}{(2\pi)^6}\frac{\rho}{2}\int v(\mathbf{k}-\mathbf{k}')\,\rho\,\gamma^2(\mathbf{k})\frac{\gamma^2(\mathbf{k}')}{1-\rho^2\gamma^2(\mathbf{k}')}\,d\underline{k}'d\underline{k}$$

The second and succeeding rows yield

$$\frac{1}{(2\pi)^6}\frac{\rho}{2}\int v(\mathbf{k}-\mathbf{k}')\,\rho^3\gamma^4(\mathbf{k})\frac{\gamma^2(\mathbf{k}')}{1-\rho^2\gamma^2(\mathbf{k}')}\,d\underline{k}'d\underline{k} \tag{145}$$

$$\frac{1}{(2\pi)^6}\frac{\rho}{2}\int v(\mathbf{k}-\mathbf{k}')\,\rho^5\gamma^6(\mathbf{k})\frac{\gamma^2(\mathbf{k}')}{1-\rho^2\gamma^2(\mathbf{k}')}\,d\underline{k}'d\underline{k} \tag{146}$$

etc.

When the results for the rows are formally summed (equations (144),(145),(146), etc.) one has for the contribution of the cluster diagrams of Figure 11 to $\langle V\rangle/N$,

$$\frac{1}{(2\pi)^6}\frac{\rho}{2}\int v(\mathbf{k}-\mathbf{k}')\left\{\rho\gamma^2(\mathbf{k})+\rho^3\gamma^4(\mathbf{k})+\ldots\right\}\frac{\gamma^2(\mathbf{k}')}{1-\rho^2\gamma^2(\mathbf{k}')}\,d\underline{k}'d\underline{k} \tag{147}$$

$$=\frac{1}{(2\pi)^3}\frac{\rho}{2}\int\left\{\frac{1}{(2\pi)^3}\int v(\mathbf{k}-\mathbf{k}')\frac{\rho\gamma^2(\mathbf{k}')}{1-\rho^2\gamma^2(\mathbf{k}')}\right\}\frac{\rho\gamma^2(\mathbf{k})}{1-\rho^2\gamma^2(\mathbf{k})}\,d\underline{k}$$

The sum of equation (143) and equation (147) yields $\left[\frac{\langle V\rangle}{N}\right]_2$, the previously omitted contributions to $\frac{\langle V\rangle}{N}$. It is

$$\left[\frac{\langle V\rangle}{N}\right]_2=\frac{1}{(2\pi)^6}\frac{\rho}{2}\int\left\{\left[\int v(\mathbf{k}-\mathbf{k}')\frac{\gamma(\mathbf{k}')}{1-\rho^2\gamma^2(\mathbf{k}')}\,d\underline{k}'\right]\cdot\frac{\gamma(\mathbf{k})}{1-\rho^2\gamma^2(\mathbf{k})}+\left[\int v(\mathbf{k}-\mathbf{k}')\frac{\rho\gamma^2(\mathbf{k}')}{1-\rho^2\gamma^2(\mathbf{k}')}\,d\underline{k}'\right]\cdot\frac{\rho\gamma^2(\mathbf{k})}{1-\rho^2\gamma^2(\mathbf{k})}\right\}d\underline{k} \tag{148}$$

The sum of equations (119), (121), (143), and (147) is the complete Hamiltonian for pair excitations:

$$\frac{\langle H\rangle}{N} = \frac{1}{2}\ \rho v(o) + \frac{1}{(2\pi)^3}\int \rho v(k)\ \frac{\gamma(k)}{1-\rho\gamma(k)}\ d\underline{k} + \frac{1}{(2\pi)^3} \tag{149}$$

$$\int \left\{ \frac{h^2}{2m}\ k^2 + \frac{\rho}{2}\ \frac{1}{(2\pi)^3}\int \rho v(k-k')\ \frac{\rho\gamma^2(k')}{1-\rho^2\ \gamma^2(k')}\ d\underline{k}' \right\} \frac{\rho\gamma^2(k)}{1-\rho^2\ \gamma^2(k)}\ d\underline{k}$$

$$+ \frac{1}{(2\pi)^3}\int \left\{ \frac{\rho}{2}\ \frac{1}{(2\pi)^3}\int v(k-k')\ \frac{\gamma(k')}{1-\rho\gamma(k')}\ d\underline{k}' \right\} \frac{\gamma(k)}{1-\rho^2\ \gamma^2(k)}\ d\underline{k}$$

Alternately this may be written as

$$\frac{\langle H\rangle}{N} = \frac{1}{2}\ \rho v(o) + \frac{1}{(2\pi)^3}\int \rho v(k)\ \frac{\gamma(k)}{1-\rho\gamma(k)}\ d\underline{k} \tag{150}$$

$$+ \frac{1}{(2\pi)^3}\left\{ \int \left[\frac{h^2}{2m}\ k^2 + \frac{\rho}{2}\ I_2(k) \right] \frac{\rho\gamma^2(k)}{1-\rho^2\ \gamma^2(k)}\ d\underline{k} \right.$$

$$\left. + \int \frac{\rho}{2}\ I_1(k)\ \frac{\gamma(k)}{1-\rho^2\ \gamma^2(k)}\ d\underline{k} \right\}$$

or

$$\frac{\langle H\rangle}{N} = \frac{1}{2}\ \rho v(o) + \frac{1}{(2\pi)^3}\int \left[\frac{\hbar^2}{2m}\ k^2 + \rho\ v(k) \right. \tag{151}$$

$$\left. + \frac{\rho}{2}\ I_2(k) \right] \frac{\rho\gamma^2(k)}{1-\rho^2\ \gamma^2(k)}\ d\underline{k}$$

$$+ \frac{1}{(2\pi)^3}\int \left[\rho v(k) + \frac{\rho}{2}\ I_1(k) \right] \frac{\gamma(k)}{1-\rho^2\ \gamma^2(k)}\ d\underline{k}$$

where

$$I_1(k) = \frac{1}{(2\pi)^3}\int v(k-k')\ \frac{\gamma(k')}{1-\rho^2\ \gamma^2(k')}\ d\underline{k}' \tag{152}$$

and

$$I_2(k) = \frac{1}{(2\pi)^3} \int v(\underline{k}-\underline{k}') \frac{\rho\gamma^2(k')}{1 - \rho^2 \gamma^2(k')} \, d\underline{k}' \tag{153}$$

Varying $\frac{\langle H \rangle}{N}$ with respect to $\gamma(k)$ yields the Euler equation

$$\frac{\left[\rho v(k) + \rho I_1(k)\right] \left[1 + \rho^2 \gamma^2(k)\right] + 2\rho\left[\frac{\hbar^2}{2m} k^2 + \rho v(k) + \rho I_2(k)\right] \gamma(k)}{\left[1 - \rho^2 \gamma^2(k)\right]^2} = 0 \tag{154}$$

Its solution is the following non-linear integral equation for $\gamma(k)$

$$\left[\rho v(k) + I_1(k)\right] \rho\gamma(k) = -\left[\frac{\hbar^2}{2m} k^2 + \rho v(k) + I_2(k)\right] + \left\{\frac{\hbar^4}{4m^2} k^4 + \frac{\hbar^2}{m} k^2 \left[\rho v(k) + I_2(k)\right] + 2\rho v(k) \left[I_2(k) - I_1(k)\right] + I_2^2(k) - I_1^2(k)\right\}^{\frac{1}{2}} \tag{155}$$

The sign of the square root was determined by the constraint, $|\rho\gamma| < 1$.

Substituting the minimizing $\gamma(k)$ from equation (154) into equation (150) leads to the following minimal form of $\frac{\langle H \rangle}{N}$:

$$\frac{\langle H \rangle}{N} = \frac{1}{2} \rho v(0) + \frac{1}{(2\pi)^3} \int \frac{\rho}{2} v(k) \gamma(k) \, d\underline{k} \tag{156}$$

$$- \frac{1}{(2\pi)^3} \int \frac{\rho}{2} \left[I_1(k) \rho\gamma(k) + 3 I_2(k)\right] \frac{\rho\gamma^2}{1 - \rho^2 \gamma^2(k)} \, d\underline{k}$$

In addition to the energy, other parameters describing the ground state, such as the pair correlation function $D(\underline{r})$ and the form factor $S(\underline{k})$, are of interest. $D(\underline{r})$ is defined by

$$D(\underline{r}) = \frac{N(N-1)}{2} \quad \frac{\int \Phi^* \Phi \;\; d\underline{r}_3 \ldots d\underline{r}_N}{\int \Phi^* \Phi \;\; d\underline{r}^N}$$

For the wave function of equation (53)

$$\Phi = \prod_{i<j}{}' \left[1 + f(r_{ij})\right] ,$$

$$D(\underline{r}) = C_{v_1}\,(r_{12}) + 2f(r_{12})\; C_{v_2}(r_{12}) + f^2(r_{12})\; C_{v_3}(r_{12}) \tag{158}$$

where the functions $C_{v_1}(r_{12})$, $C_{v_2}(r_{12})$, and $C_{v_3}(r_{12})$ are those defined earlier. Summing up the terms in the cluster expansions as before, yields

$$D(\underline{r}) = 1 + 2J_3(\underline{r}) + J_1{}^2(\underline{r}) + J_2{}^2(\underline{r}) \tag{159}$$

where

$$J_1(\underline{r}) = \frac{1}{(2\pi)^3} \int \frac{\gamma(\underline{k})}{1 - \rho^2\, \gamma^2(\underline{k})} \; e^{i\underline{k}\cdot\underline{r}}\, d\underline{k} \tag{160}$$

$$J_2(\underline{r}) \quad \frac{1}{(2\pi)^3} \int \frac{\rho\gamma^2(\underline{k})}{1 - \rho^2\, \gamma^2(\underline{k})} \; e^{i\underline{k}\cdot\underline{r}}\, d\underline{k} \tag{161}$$

$$J_3(\underline{r}) \quad \frac{1}{(2\pi)^3} \int \frac{\gamma(\underline{k})}{1 - \rho\gamma(\underline{k})} \; e^{i\underline{k}\cdot\underline{r}}\, d\underline{k} \tag{162}$$

For γ (k) given by equation (113) of the last section and equivalent to that of Lee, Huang, and Yang (39) for the pseudopotential, the behavior of D(R) is

$$D(r) = 1 + O\,(1/r^4) \;, \quad (r \rightarrow \infty) \tag{163}$$

$$D(r) = (1 - a/r)^2 + O(a/r_o),\; r << r_o,\; (\rho\, g_1)^{\frac{1}{2}}\, r_o = (8\pi\rho\, a)^{\frac{1}{2}} r_o = 1 \tag{164}$$

In general, portions of the behavior of D(r) are indicated by

$$D(o) = -1 + [1 - J_1(o)]^2 + [1 + J_2(o)]^2 \tag{165}$$

and

$$D(\underline{r}) = 1 - \left\{ \frac{2 \frac{\partial \gamma(k)}{\partial k}}{\pi^2 \rho [1 - \rho\gamma(o)]^2} k = 0 \right\} \frac{1}{r^4} + 0\left(\frac{1}{r^6}\right), \quad (r \to \infty) \tag{166}$$

From this latter equation, one may see that for the $\gamma(k)$ of equation (113), equation (163), is more accurately

$$D(r) = 1 - \frac{1}{\rho^2 \pi^2 \sqrt{8\pi\rho a}} \quad \frac{1}{r^4} + 0\left(\frac{1}{r^6}\right), \quad (r \to \infty) \tag{167}$$

Another quantity descriptive of the ground state is the form factor $S(\underline{k})$

$$S(\underline{k}) = 1 + \rho \int [D(\underline{r}) - 1] \; e^{-i\underline{k}\cdot\underline{r}} \, d\underline{r} \tag{168}$$

This particular quantity is of interest because it is accessible from experimental neutron and X-ray scattering measurements (40). Using equation (159) for $D(\underline{r})$, one has

$$S(\underline{k}) = 1 + \rho \int [2J_3(\underline{r}) + J_1^2(\underline{r}) + J_2^2(\underline{r})] \; e^{-i\underline{k}\cdot\underline{r}} \, d\underline{r} \tag{169}$$

or

$$S(\underline{k}) = 1 + \frac{2\rho\gamma(k)}{1 - \rho\gamma(k)} + \frac{\rho}{(2\pi)^3} \int \left\{ \left[\frac{\gamma(k')}{1 - \rho^2\gamma^2(k')} \right] \left[\frac{\gamma(k-k')}{1 - \rho^2\gamma^2(k-k')} \right] + \rho^2 \left[\frac{\gamma^2(k')}{1 - \rho^2\gamma^2(k')} \right] \left[\frac{\gamma^2(k-k')}{1 - \rho^2\gamma^2(k-k')} \right] \right\} d\underline{k}'$$

$$= 1 + \frac{2\rho\gamma(\mathbf{k})}{1 - \rho\gamma(\mathbf{k})} + \frac{\rho}{(2\pi)^3}\int\left\{\frac{\gamma(\mathbf{k}')\quad\gamma(\mathbf{k}-\mathbf{k}')}{\left[1 - \rho^2\ \gamma^2(\mathbf{k}')\right]\left[1 - \rho^2\ \gamma^2(\mathbf{k}-\mathbf{k}')\right]}\right\} \tag{170}$$

$$\left\{1 + \rho^2\ \gamma(\mathbf{k}')\ \ \gamma(\mathbf{k}-\mathbf{k}')\right\}\ d\underline{k}$$

Another quantity of interest is the number of particles in the ground state. As stated in the last chapter, the crucial point in treating the Bose particles with repulsive interactions is that one expects a finite fraction of particles in the free particle ground state, even with the interactions turned on. This adds to the interest in it. The fraction is $\frac{N_o}{N} = \frac{N - N_{k\neq o}}{N}$ or $\frac{N_o}{N} = 1 - \frac{N_{k\neq o}}{N}$. But $N_{k\neq o}$ is defined by $\frac{N_{k\neq o}}{N} = \int \rho\, n_{k\neq o}\, d\underline{k}$ and $n_{k\neq o}$ by

$$\frac{\langle T\rangle}{N} = \frac{\hbar^2}{2m}\int k^2 n_{k\neq o}\ d\underline{k}\ . \tag{171}$$

Comparing equation (170) with equation (119), one sees that, for pair excitations,

$$n_{k\neq o} = \frac{1}{(2\pi)^3}\quad\frac{\rho\gamma^2(\mathbf{k})}{1 - \rho^2\ \gamma^2(\mathbf{k})} \tag{172}$$

and

$$\frac{N_{k\neq o}}{N} = \frac{1}{(2\pi)^3}\int\frac{\rho^2\ \gamma^2(\mathbf{k})}{1 - \rho^2\ \gamma^2(\mathbf{k})}\quad d\underline{k} \tag{173}$$

Thus,

$$\frac{N_o}{N} = 1 - \frac{1}{(2\pi)^3}\int\frac{\rho^2\ \gamma^2(\mathbf{k})}{1 - \rho^2\ \gamma^2(\mathbf{k})}\quad d\underline{k} \tag{174}$$

and the density of particles in the ground state,

$$\rho_o = \rho - \frac{1}{(2\pi)^3} \int \frac{\rho^2 \gamma^2(\underline{k})}{1 - \rho^2 \gamma^2(\underline{k})} \, d\underline{k} \qquad (175)$$

The above results may be compared with those obtained by field-theoretic methods in momentum space using the pair excitation <u>ansatz</u>

$$\Phi_p = \sum_{j=o}^{[N/2]} \sum_{k_1 \ldots k_j \neq o} A_j(k_1 \ldots k_j) \left[\prod_{\ell=1}^{j} a^+_{\underline{k}_\ell} a^+_{-\underline{k}} \right] a_o^{2j} \, \Phi^{(o)} \qquad (176)$$

with $A_j(k_1 \ldots k_j)$ representing the probability amplitude and $a_{\underline{k}}$ and $a_{\underline{k}}$ have their usual meaning as the creation and destruction operators for free bosons of momentum $\underline{k}$. This Φ_p differs from the unperturbed free particle ground state, $\Phi^{(o)}$, by excitation of particles from zero momentum to only pairs of equal and opposite momentum. Using this <u>ansatz</u> (41), one obtains for the expectation value per particle of the Hamiltonian to be used in the variational approach, an expression which is equivalent to equation (175) with the exception that in one place, ρ is replaced ρ_o,

$$\rho_o = \rho - \frac{1}{(2\pi)^3} \int \frac{\rho^2(\underline{k})}{1 - \rho^2 \gamma(\underline{k})} \, d\underline{k} \qquad (177)$$

The resulting expression in the same notation as equation (151) is

$$\frac{\langle H \rangle}{N} = \frac{1}{2} \rho v(o) + \frac{1}{(2\pi)^3} \left[\frac{\hbar^2}{2m} k^2 + \rho_o v(\underline{k}) \right. \qquad (178)$$

$$\left. + \frac{\rho}{2} I_2(\underline{k}) \right] \frac{\rho \gamma^2(\underline{k})}{1 - \rho^2 \gamma^2(\underline{k})} \, d\underline{k} + \frac{1}{(2\pi)^3} \int \left[\rho_o v(\underline{k}) \right.$$

$$\left. + \frac{\rho}{2} I_1(\underline{k}) \right] \frac{\gamma(\underline{k})}{1 - \rho^2 \gamma^2(\underline{k})} \, d\underline{k}$$

In their derivation, the limiting processes $N \rightarrow \infty$, $V \rightarrow \infty$, and $N/V \rightarrow \rho$, a finite non-zero constant, were made and those terms yielding no contribution in these limits were neglected. This same procedure is implicit in the cluster expansion approach and was mentioned earlier. Substitution of the minimizing solution $\gamma(k)$ into equation (178) leads to the following minimal form of $\frac{\langle H \rangle}{N}$.

$$\frac{\langle H \rangle}{N} = \frac{1}{2} \rho v(o) + \frac{1}{(2\pi)^3} \int \frac{\rho_o v(k)}{2} \gamma(k) \, d\underline{k} \tag{179}$$

$$- \frac{1}{(2\pi)^3} \int \frac{\rho^2 \gamma^2}{2(1 - \rho^2 \gamma^2)} \left[\rho I_1(k) \gamma(k) + 3I_2(k) - I_1(o) - I_2(o) \right] d\underline{k}$$

Some of the other previously calculated parameters of the ground state are in agreement with those obtained through field theoretic methods for the pair-excitation *ansatz* with the exception of the presence of ρ_o. Among these is the pair correlation function $D(\underline{r})$, defined by

$$D(\underline{r}) = \frac{N(N-1)}{2} \frac{\int \Phi^* \Phi \, d\underline{r}_3 \cdots d\underline{r}_N}{\int \Phi^* \Phi \, d\underline{r}^N}$$

and calculated using the wave function $\Phi = \prod'_{i<j} \left[1 + f(r_{ij})\right]$ and cluster expansions in equation (159). Proceeding through momentum space, Lee, Huang, and Yang (42), and Girardeau and Arnowitt (43) obtain (in the same notation as equation (159))

$$D(\underline{r}) = 1 + 2 \frac{\rho_o}{\rho} J_3(\underline{r}) + J_1^2(\underline{r}) + J_2^2(\underline{r}) \tag{181}$$

where $J_1(\underline{r})$, $J_2(\underline{r})$ and $J_3(\underline{r})$ were defined in equation (160), equation (161) and equation (162).

If the form of $D(\underline{r})$ as given in equation (159) is again considered, the following criticism of $D(\underline{r})$ by Girardeau and Arnowitt is important to note.

"One can show that $D(\underline{r}) \geq 1 - 2(\rho_o/\rho)^2$. Hence it is only possible for $D(\underline{r})$ to become small for small r (as it must for the true ground state if there is a strong short-range repulsion) if $\rho_o/\rho > 1/\sqrt{2}$. Furthermore, one sees that $D(o) > 0$ for $(\rho_o/\rho) < 1$. We conclude that for interparticle interactions such as the hard-sphere one, our wave function and pair correlation function become physically unrealistic for small particle separations unless $(\rho_o/\rho) \sim 1$. This tendency of $D(\underline{r})$ to increase as $r \to o$ seems to be a general defect of pair excitation states (in equation (164) $D(\underline{r})$ becomes positively infinite as $r \to o$,) and can probably only be corrected by going beyond the pair-excitation ansatz of equation (176) so as to take into account excitation of momentum-conserving groups of more than two particles." (44)

One is well aware of this failing when proceeding in configuration space, since the wave function employed for pair excitations $\Phi = \prod'_{i<j}(1 + f(r_{ij}))$ can vanish only approximately inside the core and hence the pair correlation function constructed from it cannot be expected to do better.

If one is now interested in obtaining the asymptotic series for the ground state energy utilizing either equation (156) or equation (179) and their related equations, it is instructive to consider first the meaning of the pair-excitation states as the eigenstates of the system. For a dilute system with hard-sphere interaction, Lee, Huang, and Yang (45) have shown that the eigenstates are of the pair-excitation form. For a system in the limit of weak coupling ($v(k) \rightarrow o$), Bogoliubov (46) has shown that the eigenstates are again of the pair-excitation form. With this in mind, one is led to consider either a low density expansion or a weak coupling expansion of the ground state energy obtained from the pair excitation states. To achieve the former, one may neglect the integrals $I_1(k)$, $I_2(k)$ and $\rho - \rho_o$ in $\langle H\rangle /N$ and accompanying expressions. Use of the pseudopotential $\frac{8 \delta a\hbar^2}{2m}$ $(\underline{r})$ $\frac{\partial}{\partial r}$ (r, equivalent) to the hard sphere interaction at low densities, in these expressions leads to

$$\frac{8\pi\rho a\hbar^2}{2m} \left[1 + \frac{128}{15\sqrt{\pi}} (\rho a^3)^{\frac{1}{2}}\right] \tag{182}$$

for the first two terms of the ground-state energy per particle in a low density expansion. The neglected terms may be shown to introduce an error of order (ρa^3). This procedure is equivalent to that of the previous section and of Lee, Huang, and Yang (47). It leads to the same results.

To achieve the latter type of expansion, one may proceed by iterating the variational integral equations. Since $\rho\gamma(k)$ approaches the Bogaliubov solution

$$\rho\gamma(k) = -1 - \frac{\frac{\hbar^2}{2m}k^2 + k\sqrt{\frac{\hbar^2}{2m}k^2 + \rho v(k)}}{\rho v(k)} \tag{183}$$

in the limit of weak coupling ($v(k) \rightarrow o$), equation (183) may be used as the first iterate, $\rho\gamma_o$ (k). If $\gamma(k)$ in equation (156) for $\frac{\langle H\rangle}{N}$ is replaced by $\gamma_o(k)$, an error of order $\lambda^{7/2}$ is caused in $\frac{\langle H\rangle}{N}$ (48) λ is the dimensionless coupling constant $\frac{v(o)}{a}$ and a is the range of the interaction. The final expansion for the ground state energy per particle, correct to third order in the coupling constant (48) is

$$\frac{1}{2}\ \rho v(o) - \frac{1}{2}\ \frac{1}{(2\pi)^3} \int \frac{\rho v^2(\underline{k})}{k^2}\, d\underline{k} + \frac{8}{15\pi^2}\ \beta^{3/2}\ v^{5/2}(o) \qquad (184)$$

$$+ \frac{1}{2}\ \frac{1}{(2\ )^6} \int \frac{\rho v(\underline{k})\quad v(|\underline{k}-\underline{k}'|)\ v(\underline{k}')}{k^2 k'^2}\ d\underline{k}' d\underline{k}$$

$$+ \frac{1}{(2\pi)^3}\ \lim_{k_c \to \infty} \int_{k_c}^{\infty} \frac{\rho^2\ v^3(\underline{k})}{k^4}\, d\underline{k} + \frac{1}{a^2}\ O\ \left((\rho a^3)^{3/2}\ \lambda^{7/2}\right)$$

Using the pseudopotential $V(r) = \dfrac{8\ \pi a\hbar^2}{2m}\ \dfrac{\delta(r)\partial}{\partial r}$ (r, for the dilute strongly-coupled hard-sphere system in the weak-coupling expansion leads to the following for the first two terms of the ground-state energy per particle

$$\frac{4\pi\rho a\hbar^2}{2m}\ \left[1 + \frac{128}{15\sqrt{\pi}}\ (\rho a^3)^{1/2}\right].$$

This is the same result as obtained previously. It is not too surprising since the weak coupling expansion was based upon iteration of the variational integral equation, commencing with the Bogaliubov function. The solution of the variational equation in low density approach is the Bogaliubov function for the potential $v(k) = \dfrac{8\ \pi a\hbar^2}{2m}$, i.e. the pseudo-potential. The weak-coupling approach thus serves as a verification and justification of the previous approach

Cluster Expansion Diagrams and Perturbation Diagrams.--One of the important features of the use of perturbation theory that has allowed so much progress to be made is the ability to sum certain selected classes of perturbation diagrams from various orders. These perturbation diagrams represent pictorially terms in the perturbation expansion for the energy, i.e., they represent diagrammatically certain matrix elements. They are not Feynman diagrams as they are to be read in the upward time sense. Excited particles are represented by solid lines and the unexcited particles by dashed lines. The vertices are momentum conserving. As an example, the diagram in Figure 12(a), represents the interaction between the unexcited particles one and two. In Figure 12(b), the two unexcited particles one and two interact and are excited into a pair with momentum $\underline{k}$ and $-\underline{k}$ respectively. (Remember momentum conservation at the vertices.) Subsequent interaction deexcites them back into the ground state. In Figure 12(c), the unexcited particles one and two are excited into a pair state of momentum $\underline{k}'$ and $-\underline{k}'$. From this intermediate state they interact to go to the excited state of momentum $\underline{k}$ and $-\underline{k}$ from which they pass back to the ground state. In Figure 12(d), the two particles two and three are excited to states with momentum $-\underline{k}$ and $\underline{k}$ respectively. Particle three interacts with the unexcited particle one, exciting one to have momentum $\underline{k}$, three being deexcited to the ground state of unexcited particles. One and two then return to the ground state. This indicates the nature of the interpretation of these diagrams. Figure 12(a) contributes to the first order of the perturbation energy. Figure 12(b) contributes to the second order and Figure 12(a) and 12(d) to the third order. The number of vertices indicates the order.

Typical cluster expansion diagrams of the type used in this chapter are illustrated in Figure 13. The link between particles i and j in configuration space is $f(r_{ij})$ or $\frac{1}{(2\pi)^3}\int \gamma(\underline{k})\, e^{i\underline{k}\cdot\underline{r}_{ij}}\, d\underline{k}$. Connection between these diagrams and the perturbation diagrams may be made as follows. Make a perturbation type expansion of $f(r_{ij})$ in powers of the

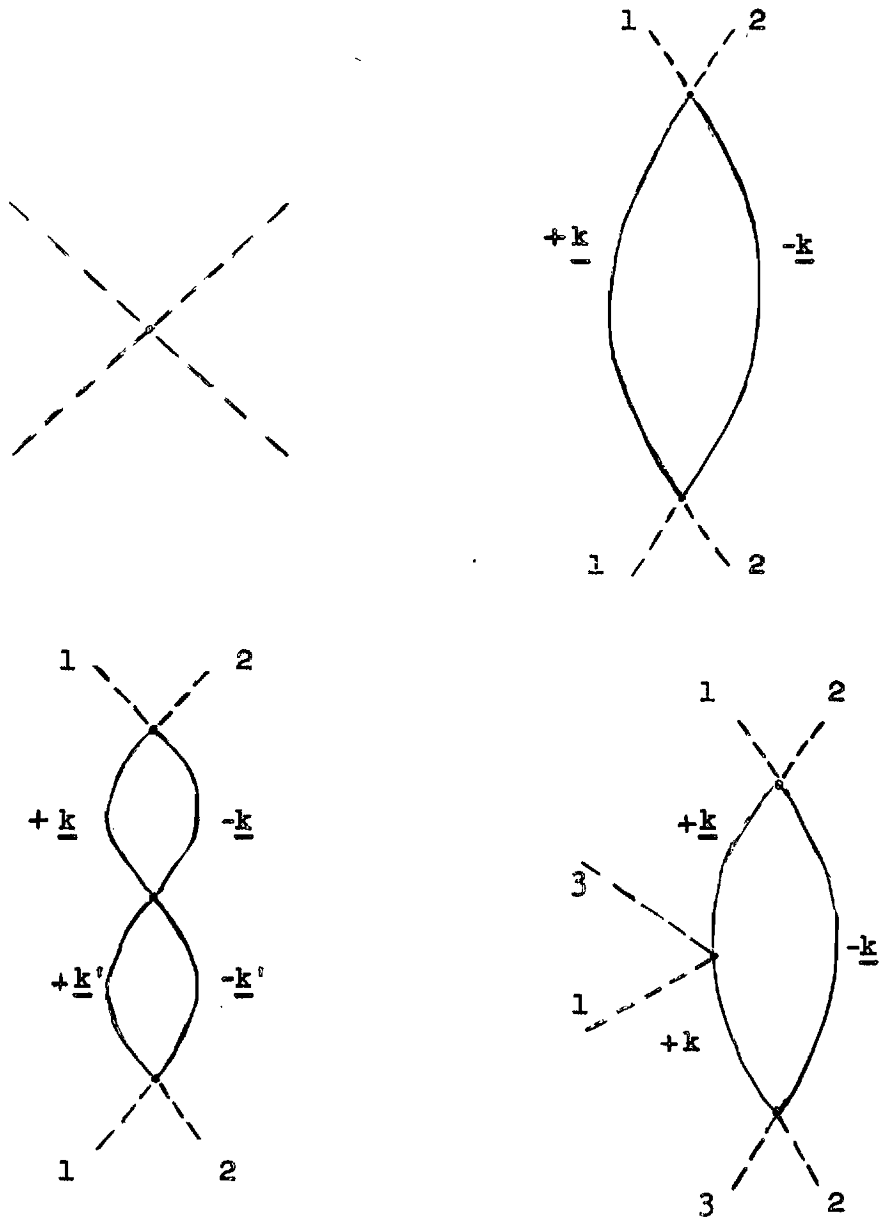


Figure 12. Typical Perturbation Diagrams

interaction strength g, i.e.

$$f(r_{ij}) = gf_1(r_{ij}) + g^2 f_2(r_{ij}) + \ldots \tag{185}$$

Alternately the Fourier transform of $f(r_{ij})$ may be so expanded, i.e.

$$\gamma(k) = \gamma_o \cdot \delta_{\underline{k},o} + \gamma_1(k)g + \gamma_2(k)\, g^2 + \ldots \tag{186}$$

where $\delta_{\underline{k},o}$ is a Kronecker-type δ. Such an expansion may be made of the solution for (k) of equation (155). It should be noted that some of the coefficients in this expansion may vanish. Then the cluster diagram of Figure 13(a) represents the interaction between the unexcited particles one and two. This is also represented by the perturbation diagram of Figure 13(a)'. The cluster diagram of Figure 13(b) for $2V(r_{12})f(r_{12})$ represents the processes shown diagrammatically in Figure 13(b)' by the series of perturbation diagrams, i.e. excitation of the pair one and two and de-excitation back to the ground state plus the iterates of this process caused by the succeeding terms in the expansion of equation (185) for $f(r_{ij})$. The cluster diagram of Figure 13(c) for $V(r_{12})\, f^2(r_{12})$ expands into the perturbation diagrams in momentum space shown in Figure 13 (c) . The sum of the two particle cluster diagrams $V(r_{12})$, $2V(r_{12})\, f(r_{12})$, and $V(r_{12})\, f^2(r_{12})$ is equivalent to the properly weighted sum of the perturbation diagrams for single pair excitations. These are illustrated in Figure 14. Retention of only these two-particle cluster diagrams leads to a reduced Hamiltonian

$$\frac{\langle H \rangle}{N} = \rho \int \left[\frac{\hbar^2}{2m}\, |\Delta\psi|^2 + \frac{V}{2}\, \psi^2 \right] d\underline{r} \tag{187}$$

The solution of its Euler equation

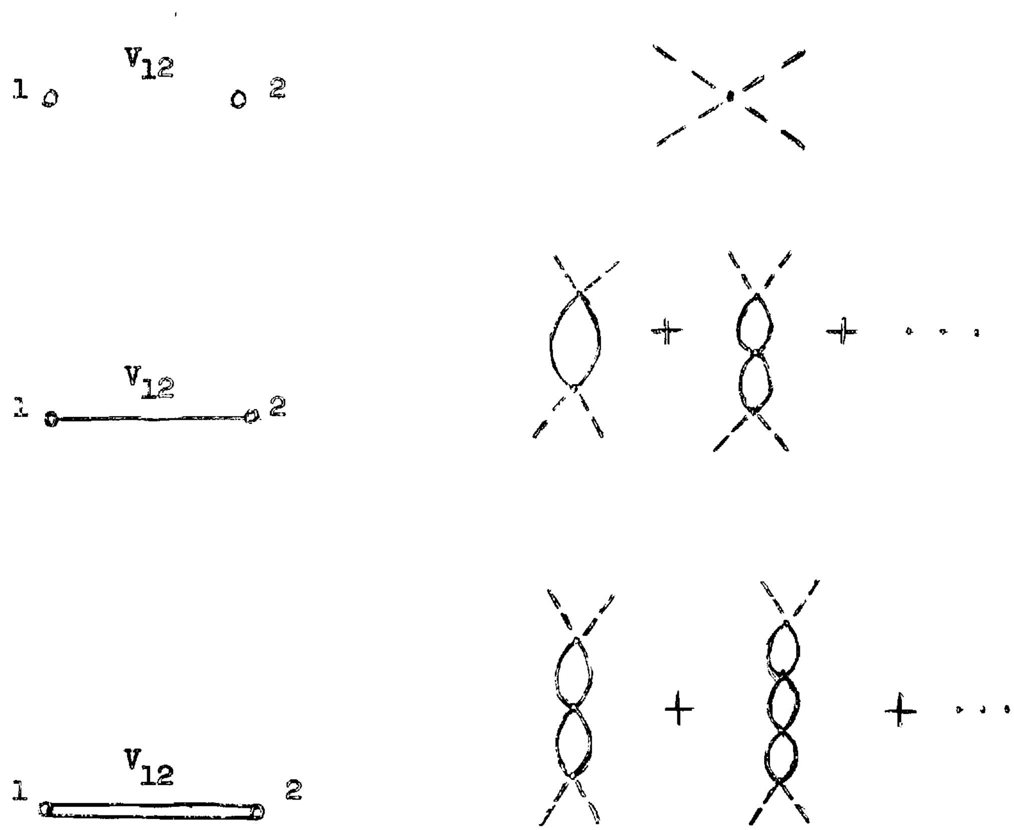


Figure 13. Two-Particle Diagrams

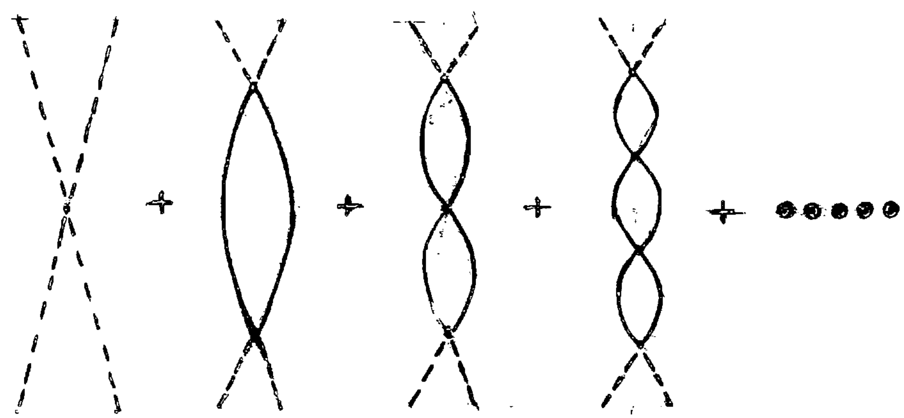


Figure 14. Single Pair Excitations

$$\frac{-\hbar^2}{2m} \quad \nabla^2 \; \psi(r) \quad \frac{1}{2} \; V(r) \; \psi(r) = 0 \tag{188}$$

for the repulsive square well of height V_o and width a is

$$\psi(r) = 1 + \frac{\alpha^{-1} \tanh \alpha a - a}{r}$$

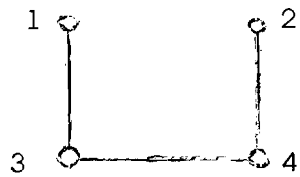
where $\alpha = \sqrt{\dfrac{mV_o}{\hbar^2}}$.

The resulting ground state energy per particle,

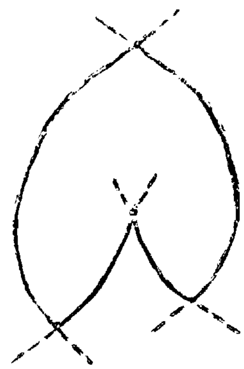
$$\frac{\langle H \rangle}{N} = \frac{4 \pi \rho \hbar^2}{2m} \left[a - \frac{\tanh \alpha a}{\alpha} \right]$$

agrees with that obtained by Abe (49). He counted only single pair excitation perturbation diagrams. It is interesting to note that the limit of this expression for the ground state energy as $V_o \rightarrow \infty$ (i.e., the repulsive square well goes into a repulsive hard core) is just the Lenz (50) term $\dfrac{4 \pi \rho a h^2}{2m}$.

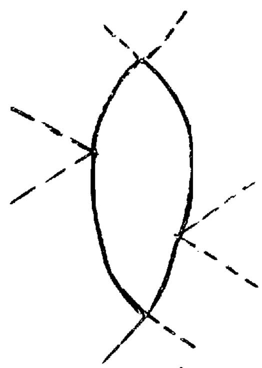
An indication of the interpretation of cluster diagrams for three or more particles in terms of perturbation diagrams for multiple pair excitations is presented in Figure (15).



$V_{12}f_{34}f_{24}f_{13}$



$V_{12}f_{13}f_{24}f_{34}$



$V_{12}f_{34}f_{24}f_{13}$

Figure 15. Typical Perturbation Diagrams Corresponding to a Particular Cluster Diagram

CHAPTER IV

CONCLUSIONS

It has been shown how the cluster integral formalism may be treated to produce results equivalent to those obtained from perturbation theory. Interest in the equivalence is not so much in presenting the cluster integral development as an alternative to the second quantization procedure; as it has been employed here at least, the cluster integral formalism appears considerably more cumbersome. Of greater interest, perhaps, is the underlying reason for the possibility of making an exact asymptotic calculation for the ground state energy in the two procedures. In the second quantization formalism, the pair approximation reduces the Hamiltonian operator from a complicated quadri-linear form in the plane wave creation and destruction operators to a simple bilinear form, which can then be diagonalized by a canonical transformation to new operators. The cluster integral formalism without the equivalent of the pair approximation is also quite intractible because of the complicated nature of admissible graphs contributing to the pair distribution function. The equivalent of the pair approximation, namely the restriction to non-repeated indices, selects out of the original hierarchy of graphs only certain ring integrals. These have a particularly simple structure which enables evaluating exactly their contribution to the pair distribution function. This fact, utilized previously in, for example, the Debye-Huckel theory of electrolytes (51), the Kahn-Uhlenback treatment of the perfect Bose-Einstein gas (52) and in the Born-Green theory of liquids (53), here again forms the basis for the possibility of the present calculation.

It has been emphasized that the properly handled cluster expansion approach has the advantage of dealing directly with the wave function in configuration space. This has the advantage of heightening one's intuition and insight into the problem.

To proceed beyond the pair excitation approximation, to include terms representing simultaneous excitation of three particles one would expect to retain terms such as $f(r_{12})\, f(r_{23})$. As previously discussed, such a term refers to excitation of three particles having momenta $\underline{k}_1$, $\underline{k}_2$, $\underline{k}_3$ with $\underline{k}_1 + \underline{k}_2 + \underline{k}_3 = 0$. However, Wu (54) has shown that instead of $f(r_{12})\, f(r_{23})$ being retained to represent a triple excitation, a term of the form $g(r_1, r_2, r_3)$ must be used. This term is not separable into the product $f(r_{12})\, f(r_{23})$, a term with a single repeated index. The implication of this for the cluster expansion approach is that for these multiple excitations to be included, a modification of the classical cluster expansions must be made to include three-body potentials in addition to the usual two-body ones.

A P P E N D I X A

DIRECT CALCULATION OF $\langle V \rangle$ FOR SINGLE PAIR EXCITATIONS

In this appendix, the result given in equation (67) for $\langle V \rangle$ the expectation value for the potential energy is derived, counting only single pair excitations, and starting from

$$I_N \langle V \rangle = I_V = \frac{1}{2} N(N-1) \int \Phi^* V(r_{12}) \Phi \, d\underline{r}^N \tag{190}$$

This amounts to calculating the integral I_V for the class of terms depicted graphically in Figures 3(a) to (d). With the ground state wave function given by equation (6), I_V becomes

$$I_V = \frac{1}{2} N(N-1) \int \prod_{i<j}' [1+f(r_{ij})] V(r_{12}) \prod_{i<j}' (1+f(r_{ij})) \, d\underline{r}^N \tag{191}$$

Contributions from terms shown in Figure 3(a) and (c) come from diagonal elements, i.e., terms in the expanded product which contain the same set of pair functions coming from Φ as from Φ^*. Call $\langle V \rangle_d$ the contribution to the potential energy from these terms. Consider the n^{th} such term, containing n products $f^2(r_{ij})$,

$$\sum f^2(r_{ij}) f^2(r_k \ ) \ldots V(r_{12}) \, d\underline{r} \tag{192}$$

Of the $N!/(N-2n)!n! \, 2^n$ terms in the sum, let $C_o(n)$ be the number in which $f^2(r_{12})$ appears and $C_1(n)$ the number in which $f^2(r_{12})$ does not appear

$$C_o(n) = \frac{(N-2)!}{[N-2-2(n-1)]!(n-1)! \, 2^{n-1}} \tag{193}$$

$$C_1(n) = \frac{N!}{(N-2n)!n! \, 2^n} - C_o(n) \ .$$

Then this n^{th} term integrated gives the result

$$\Omega^{N-n}\, C_o(n) B^{n-1} \int f(r)\, V(r) f(r)\, d\underline{r} + \Omega^{N-n}\, C_1(n) B^n \frac{\int V(r)\, d\underline{r}}{\Omega} \tag{194}$$

where $B = \int f^2(r)\, d\underline{r}$. Summing over all n, the contribution I_{vd} to I_v is

$$I_{vd} = \frac{\Omega^N}{2} \sum_{n=o}^{N/2} \frac{N!\, x^{n-1}}{(N-2n)\,!\,n!\, N^n} \;\; \frac{N(N-1)}{\Omega} \int V(r)\, d\underline{r} + \frac{\Omega^N}{2} \sum_{n=1}^{N/2} \frac{N!\, x^{n-1}}{(N-2n)\,!\,(n-1)!\, N^n}\, \rho \int f(r) V(r) f(r)\, d\underline{r} \tag{195}$$

Dividing by the normalization integral I_N

$$I_N = \Omega^N \sum_{n=o}^{N/2} \frac{N!\, x^n}{(N-2n)\,!\,n!\, N^n} \tag{196}$$

gives the result

$$\langle V \rangle_d = \frac{\rho(N-1)}{2} \int V(r)\, d\underline{r} + \frac{\rho}{2} \int f^2(r) V(r)\, d\underline{r}\, \frac{\partial}{\partial x} \log \sum_{n=o}^{N/2} \frac{N!\, x^n}{(N-2n)!\,n!\,N^n} \tag{197}$$

With the asymptotic value for the sum given by equation (60) this becomes

$$\langle V \rangle_d = \frac{N}{2} \int V(r)\, d\underline{r} \quad \frac{N\rho}{2} \int V(r)\, f^2(r)\, d\underline{r} \tag{198}$$

The second term on the right of equation (198) referring to interaction between excited pairs is neglected in this direct calculation because it affects the ground state energy in a higher order.

To complete the calculation of $\langle V \rangle$, the "off diagonal" elements, $\langle V \rangle_{od}$, coming from terms represented graphically in Figure 3(b) and (d) are needed. For the excitation and de-excitation of a pair represented in

(b) a typical n^{th} term is

$$\int f(r_{12})\ V(r_{12}) \sum f^2(r_{ij})\ f^2\ (r_{k\ell})\ \ldots\ f^2(r_s\ )\ d\underline{r}^N \tag{199}$$

with $n-\ell$ products of function $f^2(r_{ij})$, and where indices 1 and 2 appear only in the term $f(r_{12})$. On integration and on summing all such terms, one has

$$\int f(r_{12})\ V(r_{12})\ d\underline{r}_1 d\underline{r}_2 \sum_{n=1}^{N/2} C(n)\ B^{n-1}\ \ \Omega^{N-n+1} \tag{200}$$

with

$$C(n) = 2\ \frac{(N-2)!}{\left[N-2-2(n-1)\right]\ !(n-1)!\ 2^{n-1}} \tag{201}$$

The integral I_{vodl} will be

$$I_{vodl} = \rho \int V(r)\ f(r)\ d\underline{r}\ \ \Omega^N \sum_{n=1}^{N/2} \frac{N!\ x^{n-1}}{(N-2n)\ \ !(n-1)!N^n} \tag{202}$$

and

$$\langle V \rangle_{odl} = \rho \int V(r)\ f(r) d\underline{r}\ \ \frac{\partial}{\partial x}\ \log \sum_{n=o}^{N/2} \frac{N!\ x^n}{(N-2n)\ !n!\ N^n} \tag{203}$$

$$= N\rho \int V(r)\ f(r)\ d\underline{r}$$

The final contribution will come from terms shown in Figure 3(d) . A typical n^{th} term in the expanded product will be

$$\int \sum f(r_{ij})\ V(r_{12})\ f(r_{2j})\ f^2(r_k\ )\ \ldots\ f^2(r_s\ )\ dr^N \tag{204}$$

with n-1 functions $f^2(r_{ij})$. On integrating and summing all such terms, one has

$$\int f(r_{ij})\ V(r_{12})\ f(r_{2j})\ d\underline{r}_1\ d\underline{r}_2\ d\underline{r}_3 \sum_{n=1}^{N-1/2} C(n)\quad \Omega^{N-n-2}\ B^{n-1} \tag{205}$$

with

$$C(n) = 2\ \frac{(N-2)!}{\left[N-3-2(n\ 1)\right]!\ (n-1)!\quad 2^{n-1}}$$

The integral I_{vod2} will be

$$I_{vod2} = \Omega^N \frac{\rho}{\Omega 2} \int f(r_{ij})V(r_{12})f(r_{2j})d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \sum_{n=1}^{N-1/2} \frac{N!\ x^{n-1}}{(N-1-2n)!(n-1)!N^n} \tag{206}$$

Putting $\ell = n - 1$ in the sum, this becomes

$$I_{vod2} = \frac{(N-1)(N-2)}{2}\ \Omega^N \int f(r_{ij})V(r_{12})d\underline{r}_1 d\underline{r}_2 d\underline{r}_3 \sum_{=0}^{N-3/2} \tag{207}$$

$$\frac{(N-3)!\ x^{\ell}}{(N-3-2\ell)!\ \ell!\ N}$$

The asymptotic value for the sum for large N and small x is

$$e^{(N-3)x} \tag{208}$$

This gives the result

$$\langle V\rangle_{od2} = \frac{N\rho^2}{\Omega} \int f(r_{ij})\ V(r_{12})\ f(r_{2j})\ d\underline{r}_1 d\underline{r}_2 d\underline{r}_j \tag{209}$$

Introducing relative coordinates $\underline{r} = \underline{r}_1 - \underline{r}_2$, $\underline{r}' = \underline{r}_2 - \underline{r}_j$.

$$\langle V\rangle_{od2} = N\rho^2 \int f(|\underline{r} + r'|)\ V(r)\ f(r')\ d\underline{r}\ d\underline{r}' \tag{210}$$

Combining equation (198), (203), and (210) gives the total contribution to $\langle V \rangle$ from single pair excitations as

$$\langle V \rangle = \frac{N\rho}{2} \int V(r)d\underline{r} + N\rho \int V(r)f(r)d\underline{r} + N\rho^2 \int f(|r+r'|)V(r)f(r')d\underline{r}d\underline{r}' \tag{211}$$

which is the result used in Chapter III, equation (67).

APPENDIX B

DERIVATION OF EQUATION (111)

In this appendix, equation (111) is derived. To do this, the sum of equation (58) and equation (67) is considered term-by-term, using for $V(r)$ the pseudopotential given by equation (24) and transforming the pair function $f(r_{12})$ to momentum space

$$f(r_{12}) = \frac{1}{(2\ )^3} \int \gamma(k)\ e^{i\underline{k}\cdot\underline{r}_{12}}\ d\underline{k} \tag{212}$$

Equation (212) is in accordance with equation (28)

$$\gamma(k) = \int f(r_{12})\ e^{-i\underline{k}\cdot\underline{r}_{12}}\ d\underline{r}_{12}$$

Considering each term of equation (58), one has

$$\frac{\rho}{2} \int V(r_{12})\ d\underline{r}_{12} = \frac{\rho}{2} \int g\,\delta(\underline{r}_{12})\ d\underline{r}_{12} = \frac{\rho g}{2} \tag{213}$$

$$\frac{\rho}{2} \int 2V(r_{12})\ f(r_{12})\ d\underline{r}_{12} = \rho \int g\,\delta(\underline{r}_{12}) \left[\frac{1}{(2\pi)^3} \int \gamma(k)\ e^{i\underline{k}\cdot\underline{r}_{12}}\ d\underline{k}\right] d\underline{r}_{12} = \frac{\rho g}{(2\ )^3} \int \gamma(k)\ d\underline{k} \tag{214}$$

$$\frac{\rho}{2} \int V(r_{12})\ \frac{2\rho}{(2\pi)^3} \left\{\int \frac{\gamma^2(k)}{1-\rho\,\gamma(k)}\ e^{i\underline{k}\cdot\underline{r}_{12}}\ d\underline{k}\right\} d\underline{r}_{12} \tag{215}$$

$$= \frac{\rho^2}{(2\pi)^3} \int g\,\delta(\underline{r}_{12}) \left\{\int \frac{\gamma^2(k)}{1-\rho\gamma(k)}\ e^{i\underline{k}\cdot\underline{r}_{12}}\ d\underline{k}\right\} d\underline{r}_{12}$$

$$= \frac{\rho^2 g}{(2\pi)^3} \int \frac{\gamma^2(k)}{1-\rho\,\gamma(k)}\ d\underline{k}$$

Consider next the first term of equation (67). As noted in the first section of Chapter III it vanishes, since $f(r_{12})$ has no zero momentum components. Hence

$$\frac{-\rho \hbar^2}{2m} \int \nabla^2 f(r_{12})\, d\underline{r}_{12} = 0 \tag{216}$$

Considering the remaining terms of equation (67), one finds

$$\begin{aligned}
&\frac{-\rho h^2}{2m} \int f(r_{12})\, \nabla^2 f(r_{12})\, d\underline{r}_{12} \qquad (217)\\
&= \frac{-\rho h^2}{2m} \int d\underline{r}_{12} \left\{ \frac{1}{(2\pi)^6} \int \gamma(k')\, e^{-i\underline{k}'\cdot\underline{r}_{12}}\, d\underline{k}' \int -k^2\ \gamma(k)\, e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \right\}\\
&= \frac{\rho h^2}{2m} \frac{1}{(2\pi)^3} \int k^2\, \gamma^2(k)\, d\underline{k}
\end{aligned}$$

$$\begin{aligned}
&\frac{-\rho 3h^2}{2m} \int \nabla^2 f(r_{12}) \left\{ \frac{1}{(2\pi)^3} \int \frac{\gamma^3(k)}{1-\rho^2\gamma^2(k)}\, e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \right\} d\underline{r}_{12} \qquad (218)\\
&= \frac{-\rho^3 h^2}{2m} \frac{1}{(2\pi)^6} \int d\underline{r}_{12} \left\{ \int -k'^2\, \gamma(k') e^{-i\underline{k}'\,\underline{r}_{12}}\, d\underline{k}' \int \frac{\gamma^3(k)}{1-\rho^2\gamma^2(k)} \right.\\
&\left. e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \right\} = \frac{\rho^3 h^2}{2m} \frac{1}{(2\pi)^3} \int \frac{k^2\gamma^4(k)}{1-\rho^2\gamma^2(k)}\, d\underline{k}
\end{aligned}$$

The summing of equations (213) through (217) results in equation (111).

A P P E N D I X C

DERIVATION OF EQUATION (119)

In this appendix, equation (119) is obtained from equation (110). To do this $V(r_{12})$ and $f(r_{12})$ are transformed to momentum space by

$$f(r_{12}) = \frac{1}{(2\pi)^3} \int \gamma(k)\, e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \tag{219}$$

and

$$V(r_{12}) = \frac{1}{(2\pi)^3} \int \nu(k)\, e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k} \tag{220}$$

Examining each term of equation (117), one has

$$\frac{\rho}{2} \int V(r_{12})\, d\underline{r}_{12} = \frac{\rho}{2}\ \nu(o) \tag{221}$$

$$\frac{\rho}{2} \int 2V(r_{12})\, f(r_{12})\, d\underline{r}_{12} = \tag{222}$$

$$= \rho\int \left[\frac{1}{(2\pi)^3} \int \nu(k')\, e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k}'\right] \left[\frac{1}{(2\pi)^3} \int \gamma(k) e^{i\underline{k}\cdot\underline{r}_{12}}\, d\underline{k}\right] d\underline{r}_{12}$$

$$= \frac{\rho}{(2\pi)^3} \int \nu(k)\ \gamma(k)\ d\underline{k}$$

$$\frac{\rho}{2} \int V(r_{12})\ \frac{2\rho}{(2\pi)^3} \left\{\int \frac{\gamma^2(k)}{1-\rho\gamma(k)}\ e^{ik\cdot\underline{r}_{12}}\, d\underline{k}\right\} d\underline{r}_{12} \tag{223}$$

$$= \frac{\rho^2}{(2\pi)^6} \int \left[\int \nu(k')\, e^{i\underline{k}'\, r_{12}}\, d\underline{k}'\right]\left[\int \frac{\gamma^2(k)}{1-\rho\gamma(k)}\ e^{i\underline{k}\cdot\underline{r}_{12}}\, dk\ \ d\underline{r}_{12}\right.$$

$$= \frac{\rho^2}{(2\pi)^3} \int \frac{\nu(k)\, \gamma^2(k)}{1-\rho\gamma(k)}\ d\underline{k}$$

The sum of equations (221) through (223) is equation (119).

APPENDIX D

THE PSEUDOPOTENTIAL

The approach of Lee, Huang, and Yang to the problem of the system of Bose hard spheres is known as the method of pseudopotentials in contrast with Lee and Yang's binary collision expansion method (55) or Brueckner and Sawada's t-matrix method (56). The use of this concept, originally due to Fermi, is essential to their calculations. Applied to the problem of the hard spheres, this method becomes a systematic procedure of expansion of the energies and wave functions of the involved system with a, the hard-sphere diameter as expansion parameter.

Motivation for the use of the pseudopotential concept may be obtained by first discussing its role in the two body problem. For two hard spheres of diameter the Schrödinger equation is

$$(\nabla^2 + k^2) \quad \psi(\underline{r}) = 0, \ r > a \tag{224}$$

with the boundary condition

$$\psi(\underline{r}) = 0, \quad r \leq a$$

Here $\underline{r}$ is the interparticle separation and $\frac{\hbar^2 k^2}{2m}$ is the energy of relative motion. The psuedopotential may be defined as the potential in a Schrödinger equation valid throughout all space whose solution is equal to the solution of the hard sphere problem in the region outside the core. In other words, the hard core boundary condition of equation has been replaced by a potential, the pseudopotential. This procedure is analogous to the introduction of multipoles in electrostatics.

First consider the case of the appropriate pseudopotential for the spherically symmetric (δ -wave) solutions at very low energy. If $\psi(r)$ extrapolated is the solution which coincides with $\psi(\underline{r})$ outside the core,

$$(\nabla^2 + k^2)\,\psi_{ex}(r) = 0 \qquad (r \neq 0) \tag{225}$$

is the equation which it satisfies. To insure that $\psi_{ex}(r)$ will equal $\psi(a) = 0$, this equation must be altered at the origin. If $\psi_{ex}(r)$ has the following behavior close to the origin

$$\psi_{ex}(r) \rightarrow \;(1 - a/r)\,\frac{\partial}{\partial r}\left[r\;\psi_{ex}(r)\right]_{r=0}\;(r \rightarrow 0) \tag{226}$$

it will vanish at r = a. For $\psi_{ex}(r)$ to have this behavior, equation (225) will require that

$$\nabla^2\;\psi_{ex}(r) \rightarrow\; 4\pi a\,\delta(\underline{r})\,\frac{\partial}{\partial r}\;(r\;\psi_{ex}(r)\;)\;(r \rightarrow 0),(k \rightarrow 0) \tag{227}$$

In this equation $\delta(\underline{r})$ has its usual meaning as a Dirac δ-function. The end result is that $\psi_{ex}(\underline{r})$ is a solution of

$$(\nabla^2 + k^2)\;\;\psi_{ex}(\underline{r}) = 4\pi a\,\delta(\underline{r})\;\;\frac{\partial}{\partial r}\;\left[r\;\;\psi_{ex}(\underline{r})\right] \tag{228}$$

but is an S-wave asymptotic solution ($k \rightarrow 0$) of the original problem for $r \geq a$. The operator on the right, being the potential of this Schrödinger equation, is called the pseudopotential. This equation is not the originally sought equation whose equation $\psi_{ex}(\underline{r})$ coincides exactly with $\psi(\underline{r})$ for $r \geq a$. Its pseudopotential correspondingly is only approximately the desired pseudopotential. To determine the desired pseudopotential. To determine the desired pseudopotential, the solution for $r \geq a$ of equation (224) will be written as

$$\psi(\underline{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-1}^{+1} A_{\ell m} Y_{\ell m}(\theta, \phi) \left[j_{\ell}(kr) - (\tan {}_{\ell}) n_{\ell}(kr) \right], \quad (229)$$

In this equation, (r, θ, ϕ) are the polar coordinates for $\underline{r}$, $Y_{\ell m}(\theta,\phi)$ is a normalized spherical harmonic, and $j_{\ell}(kr)$ and $n_{\ell}(kr)$ are spherical Bessel functions. The η_{ℓ}, phase shifts for scattering from a hard sphere are defined by

$$\tan \eta_{\ell} = \frac{j_{\ell}(ka)}{n_{\ell}(ka)} \quad . \quad (230)$$

This is the solution of equation (224) for $r \geq a$. If $\psi_{ex}(\underline{r})$ is defined to be equal to this expression throughout all space, then one may show that the equation it satisfies is

$$(\nabla^2 + k^2) \quad \psi_{ex}(\underline{r}) = \frac{4\pi}{-kc_o + \eta_o} \quad \delta(\underline{r}) \frac{\partial}{\partial r} \quad (r \quad \psi_{ex}(r) \quad (231)$$

$$+ \sum_{\ell=1}^{\infty} \sum_{m=-1}^{+1} \left\{ \frac{-\tan \eta_{\ell}}{k^{2\ell+1}} \quad \frac{(2\ell-1)!!\,(\ell+1)}{!\,2^{\ell}} \right.$$

$$Y_{\ell m} \left[\frac{\delta(\underline{r})}{r^{\ell+2}} \quad \left(\frac{d}{dr}\right)^{2\ell+1} (r^{\ell+1} \quad \psi_{\ell m}) \right.$$

In this equation, $\psi_{\ell m}$ is defined by

$$\psi_{\ell m} = \int Y^{*}_{\ell m}(\theta, \phi) \, \psi(\underline{r}) \, d\Omega$$

The derivation shows that "in general, the solution of equation (225) yeilds the correct eigenvalues and correct asymptotic wave functions for any potential without bound states. The hard sphere potential is a particularly simple case in which the asymptotic form is realized as soon as $r \geq a$." (57)

In this consideration of the two-body problem, the two-body pseudopotential replaced the hard-sphere boundary condition that ψ vanish whenever $|\underline{r}_1 - \underline{r}_2| \leq a$. This means that ψ must vanish on and inside a tube of radius a in the 6 dimensional configuration space of the two particles. The tube axis is defined by $|\underline{r}_1 - \underline{r}_2| = 0$. In the case of the N-body system, this boundary condition becomes the requirement that ψ vanish whenever $|\underline{r}_i - \underline{r}_j| \leq a$ for all i and j, i different from j. This means that ψ must vanish on and inside tubes of radius a, one tube for each different pair of particles i, j in the 6N dimensional configuration space of the problem. The axis of each tube is defined by $|\underline{r}_i - \underline{r}_j| = 0$, the surface by $|\underline{r}_i - \underline{r}_j| \leq a$. The collection of all $\frac{N(N-1)}{2}$ tubes is a tree-like hyper surface, the tubes mutually intersecting to form the center. A given tube, say one defined by $|\underline{r}_i - \underline{r}_j| = a$, may be replaced correctly in a region removed from any intersections by the corresponding two-body pseudopotential. Thus away from intersections of two or more tubes the extended or extrapolated wave function would be a solution of a Schrödinger equation containing the sum of $\frac{N(N-1)}{2}$ two-body pseudopotentials. To determine the pseudopotentials required by the intersection of two or more tubes would require the solution of three and more-body problems. Instead of doing this, Lee, Huang, and Yang use for the N-body pseudopotential the approximation

$$\frac{8\pi a\hbar^2}{2m} \sum_{i<j} \delta(\underline{r}_i - \underline{r}_j) \frac{\partial}{\partial r_{ij}} (r_{ij} \tag{233}$$

which is valid to order a^2. This approximation amounts to using the sum of the first term of the two-body pseudopotentials.

A P P E N D I X E

ASYMPTOTIC SERIES: NOTATION AND DISCUSSION

The meaning of the O and o notation is found through the following definitions:

1. If S is any set and f and g are functions defined on it, then

$$f(s) = O\left[g(s)\right], \qquad s$$

means that there exists a positive number A, independent of s, such that

$$f(s) \leq A\, g(s) \quad \text{for all } s$$

2. If f and g are functions defined on the real line, then

$$f(x) = O\left[g(x)\right], \quad (x \rightarrow$$

means that there exists a real number k such that

$$f(x) = O\left[g(x)\right], \quad x \quad (k, \quad) .$$

3. If f and g are functions defined on a set S, then

$$f(x) = O\left[g(x)\right], \quad (x \rightarrow x_0)$$

means that there exists a positive constant A and a neighborhood $N(x_0)$ of x_0 such that

$$f(x) \leq A \; g(x) \quad \text{for all } x \quad \text{both } s \text{ and } N(x_0),$$

4. If f and g are functions defined on a set S, then

$$f(x) = O\left[g(x)\right], \ (x \rightarrow x_0)$$

means that $f(x)/g(x) \rightarrow 0$ as $x \rightarrow x_0$.

To say that $h(x)$ is an "asymptotic formula for $f(x)$" or that "$f(x)$ and $g(x)$ are asymptotically equivalent" $[f(x) \sim g(x)]$ means that

$$f(x)/g(x) \to 1 \text{ as } x \to x_o .$$

The preceding definitions are now used to define what is meant by an "asymptotic series for $f(x)$" or "an asymptotic expansion of $f(x)$."

If there exists a sequence of functions h_o, h_1, h_2, h_3,... and if there exists a sequence of constants C_o, C_1, C_2,... such that this series of O-formulas for $f(x)$ holds:

$$f(x) = O\left[h_o(x)\right], \qquad (x \to x_o)$$

$$f(x) = C_o h_o(x) + O\left[h_1(x)\right], \qquad (x \to x_o)$$

$$f(x) = C_o h_o(x) + C_1 h_1(x) + O\left[h_2(x)\right], \qquad (x \to x_o)$$

$$f(x) = C_o h_o(x) + \dots + C_{n-1} h_{n-1}(x) + O\left[h_n(x)\right], \quad (x \to x_o)$$

then the formal series

$$C_o h_o(x) + C_1 h_1(x) + \dots, \qquad (x \to x_o)$$

is an "asymptotic series for $f(x)$" and the following notation is used

$$f(x) = C_o h_o(x) + \dots, \qquad (x \to x_o)$$

and includes the set of O-formulas. If this set has only N members, then it is said to be an asymptotic expansion of $f(x)$ to N-1 terms.

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