

unit volume is approximately given by

$$P = J_x E_x + J_y E_y + J_z E_z.$$

### Transport Properties

Equations (15) expresses the thermal and electrical currents in terms of temperature gradient, electric

field and magnetic field. Expressions for transport properties may be found by using suitable sets of auxiliary conditions.

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## Cluster Integrals and the Ground State of Bosons with Repulsive Interactions

H. A. GERSCH AND V. H. SMITH

*School of Physics, Georgia Institute of Technology, Atlanta, Georgia*

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The properties of a Bose system of particles with repulsive interactions have previously been treated using perturbation theory in the formalism of second quantization. Others have also considered this problem by dealing with the wave function in configuration space, using the theory of cluster expansions. In these latter papers, variation with respect to a parameter in a trial function for the ground state has been shown to yield a ground-state energy close to the exact asymptotic expressions obtained from perturbation theory. The connection between the two methods is not immediately obvious from these cluster expansion treatments. It is shown here that, as one might expect, the cluster integral method can be handled so that it is completely equivalent to the pair approximation in perturbation theory.

### 1. INTRODUCTION

THE properties of a Bose system of particles with repulsive interactions has been treated using the formalism of second quantization by several investigators.<sup>1-3</sup> More recently<sup>4,5</sup> 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.<sup>6</sup> 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 at low densities 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 references 2 and 3 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.<sup>7</sup> One might expect that here as well, the pair approximation perturbation theory should have its exact counterpart in a configuration space cluster integral development. Our purpose 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. The pair approximation yields a ground state which in configuration space has the form [see Eq. (A.21) of Appendix II of reference 3]

$$\Psi = \prod'_{i < j=1}^N [1 + f(r_{ij})], \quad (1)$$

where the prime denotes that in the expanded product for  $\Psi$  all terms with repeated particle indices are omitted. The prohibition of repeated indices is essential for the pair 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  $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$  with  $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = 0$ .<sup>3</sup> The previous cluster integral developments do not

<sup>1</sup> N. N. Bogoliubov, *J. Phys. (U.S.S.R.)* **2**, 23 (1947).

<sup>2</sup> K. A. Brueckner and K. Sawada, *Phys. Rev.* **106**, 1117 (1957).

<sup>3</sup> T. D. Lee, K. Huang, and C. N. Yang, *Phys. Rev.* **106**, 1135 (1957).

<sup>4</sup> F. Iwamoto, *Progr. Theoret. Phys. (Kyoto)* **19**, 597 (1958).

<sup>5</sup> J. B. Aviles, *Ann. Phys.* **5**, 251 (1958).

<sup>6</sup> J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1950), Chap. 13.

<sup>7</sup> B. Kahn and G. E. Uhlenbeck, *Physica* **5**, 399 (1938).

impose this constraint of nonrepeated indices in the ground-state wave function. As a result, they 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 calculation, and hence, not directly comparable. With the constraint of nonrepeated indices, the cluster integral development becomes equivalent to the pair 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. This is demonstrated in the next section.

## 2. CLUSTER EXPANSIONS AND RING INTEGRALS

Our aim 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

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

where  $d\mathbf{r}^N = d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N$ , and  $V(r_{ij})$  is the two-body potential energy. The ground-state wave function  $\Psi$  will finally be written in the form of Eq. (1), but for the present we write it as a product of pair functions with no constraint,

$$\Psi = \prod_{i < j=1}^N [1 + f(r_{ij})] = \prod_{i < j=1}^N \psi(r_{ij}). \quad (3)$$

The cluster integrals are introduced by first reducing the multidimensional integral in Eq. (2) 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<sup>5</sup>

$$\begin{aligned} \frac{\langle H \rangle}{N} = & -\frac{\rho \hbar^2}{2m} \int \left\{ [\psi(r_{12}) \nabla^2 \psi(r_{12})] C(r_{12}) \right. \\ & + \frac{1}{2} \psi(r_{12}) \nabla \psi(r_{12}) \cdot \nabla C(r_{12}) \\ & \left. - \frac{m}{\hbar^2} V(r_{12}) \psi^2(r_{12}) C(r_{12}) \right\} d\mathbf{r}_{12}, \quad (4) \end{aligned}$$

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

$$C(r_{12}) = \frac{N(N-1)}{\rho^2 \psi^2(r_{12})} \int \prod_{i < j=1}^N \psi^2(r_{ij}) d\mathbf{r}_3 \cdots d\mathbf{r}_N / \int \prod_{i < j=1}^N \psi^2(r_{ij}) d\mathbf{r}_1 \cdots d\mathbf{r}_N, \quad (5)$$

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

$$\rho^2 \psi^2(r_{12}) C(r_{12}) = n_2(r_{12}). \quad (6)$$

The function  $C(r_{12})$  can be expressed in a cluster expansion in powers of the density<sup>8</sup>

$$C(r_{12}) = 1 + \sum_{n=1}^{\infty} \rho^n \xi_n(r_{12}), \quad (7)$$

where

$$\xi_n(r_{12}) = \frac{1}{n!} \int \sum \prod h(r_{ij}) d\mathbf{r}_3 \cdots d\mathbf{r}_{n+2}, \quad (8)$$

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

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. The potential energy contribution is given by

$$\frac{\langle V \rangle}{N} = \frac{\rho}{2} \int V(r_{12}) \psi^2(r_{12}) C(r_{12}) d\mathbf{r}_{12}. \quad (9)$$

Without the restriction of nonrepeated indices on the ground-state wave function, the evaluation of the integrals in Eq. (9) corresponding to clusters of considerable numbers of particles becomes prohibitively difficult. However, the nonrepeated indices requirement 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 modified by the hypothesis of nonrepeated indices. Since  $\psi(r_{ij}) = 1 + f(r_{ij})$ , we can write Eq. (9) in the form

$$\begin{aligned} \frac{\langle V \rangle}{N} = & \frac{\rho}{2} \int \{ V(r_{12}) C_{V1}(r_{12}) + 2V(r_{12}) C_{V2}(r_{12}) f(r_{12}) \\ & + V(r_{12}) f^2(r_{12}) C_{V3}(r_{12}) \} d\mathbf{r}_{12}. \quad (10) \end{aligned}$$

We examine first the cluster expansion of  $C_{V1}(r_{12})$ :

$$C_{V1}(r_{12}) = 1 + \sum_{n=1}^{\infty} \rho^n \xi_{n1}(r_{12}), \quad (11)$$

where

$$\xi_{n1}(r_{12}) = \frac{1}{n!} \int \sum_{(1)} \prod h(r_{ij}) d\mathbf{r}_3 \cdots d\mathbf{r}_{n+2}, \quad (12)$$

and the integrand  $\sum_{(1)} \prod h(r_{ij})$  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 and only those connected products are allowed which are consistent with the assumption of nonrepeated indices in  $\Psi$ . As a first consequence of the latter, only ring-connected products are allowed. Those connected products with internal connections are not

<sup>8</sup> See, e.g., J. deBoer, *Reports on Progress in Physics* (The Physical Society, London, 1948-49), Vol. 12, p. 335.

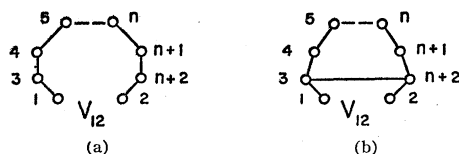


FIG. 1. Graphs representing contributions to the ground-state energy. (a) A typical connected product. (b) A connected product not allowed by the requirement of nonrepeated indices.

involved. For example a ring product such as is illustrated in Fig. 1(a) is allowed, whereas a product with an internal connection [such as is illustrated in Fig. 1(b)] would imply the existence of repeated indices in  $\Psi$ . We further note that the  $f^2(r_{ij})$  term in  $h(r_{ij})$  is eliminated by the assumption of nonrepeated indices. In the cluster expansion where repeated indices are allowed, the factor  $2f(r_{ij})$  in Eq. (8) for  $h(r_{ij})$  indicates that there are two places in any cluster from which each  $f(r_{ij})$  may come, i.e., from  $\Psi$  or  $\Psi^*$ . In our case of nonrepeated indices, this particular degeneracy is not present. For example, a ring of order  $n=3$  contains the product  $f(r_{13})f(r_{34})f(r_{45})f(r_{52})V(r_{12})$ . The pair functions  $f(r_{13})$  and  $f(r_{45})$  may come from  $\Psi$  while  $f(r_{34})$  and  $f(r_{52})$  must then come from  $\Psi^*$ . Thus,

$$\xi_{n1}(r_{12}) = \frac{1}{n!} \sum \prod f(r_{ij}) d\mathbf{r}_3 \cdots d\mathbf{r}_{n+2}. \quad (13)$$

All the connected ring products illustrated in Fig. 2 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, we include only those connected products in the first row of Fig. 2.

To evaluate  $\xi_{n1}(r_{12})$ , note that permuting the  $n$  particles produces  $n!$  configurations, while there are also two ways of drawing the configuration from  $\Psi$  and

$\Psi^*$ . Hence,

$$\sum \prod f(r_{ij}) = 2(n!) f(r_{13}) f(r_{34}) \cdots \times f(r_{n+1, n+2}) f(r_{n+2, 2}), \quad (14)$$

and

$$\xi_{n1}(r_{12}) = 2 \int f(r_{13}) f(r_{34}) \cdots f(r_{n+2, 2}) d\mathbf{r}_3 \cdots d\mathbf{r}_{n+2}. \quad (15)$$

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

$$\gamma(k) = \int f(r) e^{-ik \cdot r} d\mathbf{r}. \quad (16)$$

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

$$\xi_{n1}(r_{12}) = \frac{2}{(2\pi)^3} \int [\gamma(k)]^{n+1} e^{ik \cdot r_{12}} d\mathbf{k}, \quad (17)$$

and thus

$$C_{V1}(r_{12}) = 1 + \frac{2}{(2\pi)^3} \sum_{n=1}^{\infty} \int [\rho \gamma(k)]^{n+1} e^{ik \cdot r_{12}} d\mathbf{k}. \quad (18)$$

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

$$C_{V1}(r_{12}) = 1 + \frac{2\rho}{(2\pi)^3} \int \frac{\gamma^2(k)}{1 - \rho \gamma(k)} e^{ik \cdot r_{12}} d\mathbf{k}. \quad (19)$$

We next consider the second term in  $\langle V \rangle / N$  given in Eq. (10), i.e.,

$$V(r_{12}) f(r_{12}) C_{V2}(r_{12}). \quad (20)$$

We note that  $C_{V2}$  may also be expanded in a cluster expansion,

$$C_{V2} = 1 + \sum_{n=1}^{\infty} \rho^n \xi_{n2}(r_{12}), \quad (21)$$

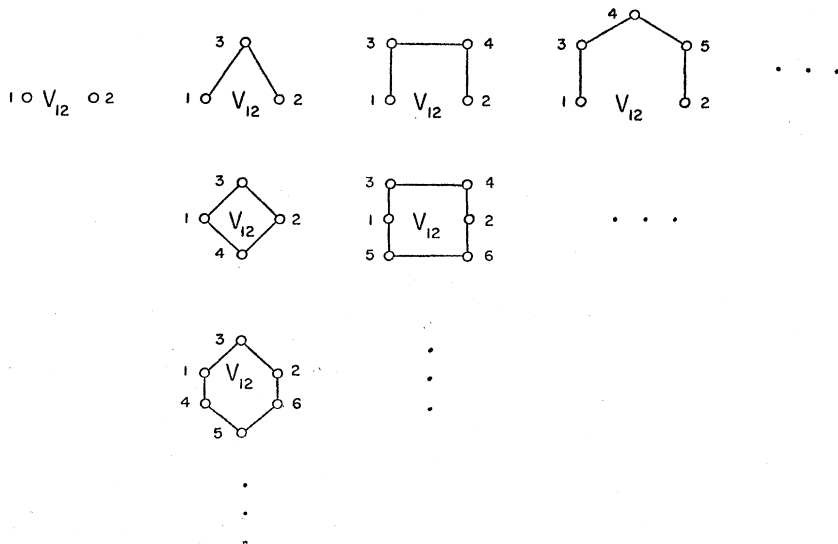


FIG. 2. Graphs representing the contributions to  $\langle V \rangle$  from the term  $V(r_{12})C_{V1}(r_{12})$  in Eq. (10).

where

$$\xi_{n2}(r_{12}) = \frac{1}{n!} \sum_{(2)} \prod f(r_{ij}) d\mathbf{r}_3 \cdots d\mathbf{r}_{n+2}, \quad (22)$$

in accordance with our previous remarks in discussing the expansion of  $C_{V1}(r_{12})$ . In this case, we are considering terms of the type  $V(r_{12})f(r_{12}) \prod f(r_{ij})$  (see Fig. 3). Nonrepeated indices require that

$$\sum_{(2)} \prod f(r_{ij}) = 0, \quad \text{for } n \text{ odd}, \quad (23)$$

and

$$\sum_{(2)} \prod f(r_{ij}) = (n!) f(r_{13}) \cdots f(r_{n+2,2}) \quad \text{for } n \text{ even}. \quad (24)$$

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

$$\begin{aligned} \xi_{n2}(r_{12}) &= 0 \quad n \text{ odd} \\ &= \frac{1}{(2\pi)^3} \int [\gamma(k)]^{n+1} e^{i\mathbf{k} \cdot \mathbf{r}_{12}} d\mathbf{k} \quad n \text{ even} \end{aligned} \quad (25)$$

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

$$C_{V2}(r_{12}) = 1 + \frac{\rho^2}{(2\pi)^3} \int \frac{\gamma^3(k)}{1 - \rho^2 \gamma^2(k)} e^{i\mathbf{k} \cdot \mathbf{r}_{12}} d\mathbf{k}. \quad (26)$$

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

$$V(r_{12}) f^2(r_{12}) C_{V3}(r_{12}).$$

Nonrepeated indices require  $C_{V3}(r_{12}) = 1$  inasmuch as one  $f(r_{12})$  must come from  $\Psi$  and the other from  $\Psi^*$ , then products which connect particles one and two are impossible. We drop this term as well as the second term in Eq. (26), since they may both be shown to contribute to a higher order in the final result for the energy.

Combining the above results, the expectation value for the potential energy per particle is

$$\begin{aligned} \frac{\langle V \rangle}{N} &= \frac{\rho}{2} \int V(r_{12}) \left( 1 + 2f(r_{12}) \right. \\ &\quad \left. + \frac{2\rho}{(2\pi)^3} \int \frac{\gamma^2(k)}{1 - \rho\gamma(k)} e^{i\mathbf{k} \cdot \mathbf{r}_{12}} d\mathbf{k} \right) d\mathbf{r}_{12}. \end{aligned} \quad (27)$$

The first term in the integral on the right side of Eq. (27) represents the interaction between unexcited particles one and two shown graphically by the first term in the first row of Fig. 2. 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 Fig. 2, corresponding to multiple pair excitations and their interaction with the unexcited particles.

The inclusion of only the integral obtained from the

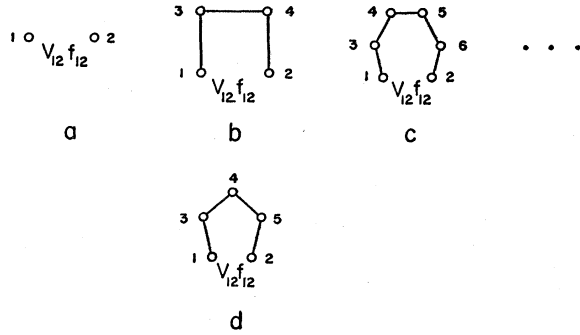


FIG. 3. (a)-(c) Graphs representing the successive contributions to  $\langle V \rangle$  from the term  $V(r_{12})f(r_{12})C_{V2}(r_{12})$  in Eq. (10). (d) A typical contribution for odd  $n$  ( $n=3$ ) which vanishes for nonrepeated indices.

first term in this series, i.e., single pair excitations and their interaction with the ground state, in a direct calculation<sup>9</sup> yields the result cited by Brueckner and Sawada.<sup>2</sup>

Now for nonrepeated indices the expectation value for the kinetic energy per particle is<sup>10</sup> from Eq. (4),

$$\begin{aligned} \frac{\langle T \rangle}{N} &= \frac{-\rho \hbar^2}{2m} \int \psi(r_{12}) \nabla^2 \psi(r_{12}) C_T(r_{12}) d\mathbf{r}_{12} \\ &= \frac{-\rho \hbar^2}{2m} \int \{ [\nabla^2 f(r_{12})] C_{T1}(r_{12}) \\ &\quad + [f(r_{12}) \nabla^2 f(r_{12})] C_{T2}(r_{12}) \} d\mathbf{r}_{12}. \end{aligned} \quad (28)$$

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

$$C_{Ti}(r_{12}) = 1 + \sum_{n=1}^{\infty} \rho^n \xi_{ni}(r_{12}), \quad (29)$$

where

$$\xi_{ni}(r_{12}) = \frac{1}{n!} \int \sum_{(i)} \prod f(r_{ij}) d\mathbf{r}_3 \cdots d\mathbf{r}_{n+2}. \quad (30)$$

Examination of these expansions (see Fig. 4) yields

$$\sum_{(1)} \prod f(r_{ij}) = 0, \quad \text{for } n \text{ odd} \quad (31)$$

$$\begin{aligned} \sum_{(1)} \prod f(r_{ij}) \\ = n! f(r_{13}) f(r_{34}) \cdots f(r_{n+2,2}) \quad \text{for } n \text{ even}, \end{aligned} \quad (32)$$

<sup>9</sup> V. H. Smith and H. A. Gersch, Bull. Am. Phys. Soc. 4, 386 (1959).

<sup>10</sup> The absence of a term  $\nabla f \cdot \nabla C$  should be noted. Such a term arises from products such as

$$\begin{aligned} \nabla^2 [f(r_{12}) f(r_{13}) f(r_{45})] \\ = \nabla_1 \cdot [f(r_{13}) f(r_{45}) \nabla_1 f(r_{12}) + f(r_{12}) f(r_{45}) \nabla_1 f(r_{13})] \\ = [\nabla^2 f(r_{12})] f(r_{13}) f(r_{45}) + f(r_{12}) f(r_{45}) \nabla_1^2 f(r_{13}) \\ + 2f(r_{45}) \nabla_1 f(r_{12}) \cdot \nabla_1 f(r_{13}) \end{aligned}$$

But such products are missing in  $\Psi$ , due to nonrepeated indices.

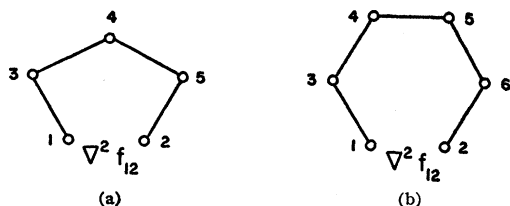


FIG. 4. Graphs representing contributions to the kinetic energy from the term  $\nabla^2 f(r_{12}) C r_1(r_{12})$  in Eq. (28). (a) A term with odd  $n$ , ( $n=3$ ) which vanishes for nonrepeated indices. (b) A term with even  $n$  ( $n=4$ ) which gives a nonvanishing contribution.

and

$$\sum_{(2)} \prod f(r_{ij}) = 0, \quad (33)$$

and thus the expectation value for the kinetic energy may finally be written as

$$\frac{\langle T \rangle}{N} = \frac{-\rho \hbar^2}{2m} \int \nabla^2 f(r_{12}) \left( 1 + f(r_{12}) + \frac{\rho^2}{(2\pi)^3} \int \frac{\gamma^3(k)}{1 - \rho^2 \gamma^2(k)} e^{ik \cdot r_{12}} d\mathbf{k} \right) d\mathbf{r}_{12}. \quad (34)$$

The expectation value for the energy per particle is then obtained by adding Eq. (27) and Eq. (34).

To make connection with the results from the perturbation theory calculation for hard spheres, we now use for  $V(r)$  the pseudopotential shown by Lee, Huang, and Yang<sup>3</sup> to be applicable to this interaction at the low densities considered here. As they have shown, it is essential, in order to remove spurious infinities, to use the correct pseudopotential,

$$V(r) = g\delta(r) (\partial/\partial r)(r), \quad g = 4\pi a \hbar^2/m, \quad (35)$$

where  $a$  is the hard sphere diameter. Actually, one can use the form  $V(r) = g\delta(r)$ , and switch to the correct form given in Eq. (35) at the end of the calculation. The expression for  $\langle H \rangle$  is considerably simplified by transforming the pair function  $f(r_{12})$  to momentum space. As shown in the Appendix, the result is

$$\frac{\langle H \rangle}{N} = \frac{\rho \hbar^2}{2m} \left( \frac{g_1}{2} + \frac{1}{(2\pi)^3} \int \frac{(k^2 + \rho g_1) \gamma^2(k) + g_1 \gamma(k)}{1 - \rho^2 \gamma^2(k)} d\mathbf{k} \right), \quad (36)$$

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

$$\frac{g_1 \rho^2 \gamma^2(k) + 2(k^2 + \rho g_1) \gamma(k) + g_1}{[1 - \rho^2 \gamma^2(k)]^2} = 0. \quad (37)$$

Its solution for  $\gamma(k)$  is

$$\rho \gamma(k) = - \left( 1 + \frac{k^2}{\rho g_1} \right) + \frac{k}{\rho g_1} (k^2 + 2\rho g_1)^{\frac{1}{2}}, \quad (38)$$

where the  $+$  sign is chosen in front of the radical to satisfy the condition that  $|\rho \gamma(k)| < 1$ . Substituting for  $\gamma(k)$  in Eq. (35) we obtain

$$\frac{\langle H \rangle}{N} = \frac{2\pi a \hbar^2 \rho}{m} \left[ 1 + \lim_{r \rightarrow 0} \frac{\partial}{\partial r} r \int \gamma(k) e^{ik \cdot r} d\mathbf{k} \right]. \quad (39)$$

Evaluating the integral yields the result

$$E_0 = \langle H \rangle = 2\pi N \rho \frac{a \hbar^2}{m} \left[ 1 + \frac{128}{15\sqrt{\pi}} (\rho a^3)^{\frac{1}{2}} \right], \quad (40)$$

which is the result previously obtained from perturbation theory.<sup>2,3</sup> Using our solution for  $\gamma(k)$ , 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 pair distribution function are also in agreement.

### 3. DISCUSSION

We have shown how the cluster integral formalism may be treated to produce results equivalent to those obtained from perturbation theory. Our interest in the equivalence is not so much in presenting the cluster integral development as an alternative to the second quantization procedure; as we have employed it 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 intractable because of the complicated nature of admissible graphs contributing to the pair distribution function. The equivalent of the pair approximation, namely the restriction to nonrepeated indices, selects out the original hierarchy of graphs only the ring integrals. These have a particularly simple structure which enables evaluating exactly their contribution to the pair distribution function. This fact, utilized previously, for example, in the Debye-Hückel theory of electrolytes,<sup>11</sup> in the Kahn-Uhlenbeck treatment of the perfect Bose-Einstein gas,<sup>7</sup> and in the Born-Green theory of liquids,<sup>12</sup> here again forms the basis for the possibility of the present calculation.

<sup>11</sup> J. E. Mayer, J. Chem. Phys. **18**, 1426 (1950).

<sup>12</sup> M. Born and H. S. Green, *A general Kinetic Theory of Liquids* (Cambridge University Press, Cambridge, 1949), Chap. II.

## APPENDIX

In this Appendix, we derive Eq. (36). To do this, we consider the sum of Eq. (27) and Eq. (34) term by term, using for  $V(r)$  the pseudopotential given by Eq. (35) and by transforming the pair function  $f(r_{12})$  to momentum space:

$$f(r_{12}) = \frac{1}{(2\pi)^3} \int \gamma(k) e^{ik \cdot r_{12}} d\mathbf{k}. \quad (\text{A1})$$

Equation (A1) is in accordance with Eq. (16)

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

Considering each term of Eq. (27), we have

$$\frac{\rho}{2} \int V(r_{12}) d\mathbf{r}_{12} = \frac{\rho}{2} \int g\delta(\mathbf{r}_{12}) d\mathbf{r}_{12} = \frac{\rho g}{2}, \quad (\text{A2})$$

$$\begin{aligned} & \frac{\rho}{2} \int 2V(r_{12}) f(r_{12}) d\mathbf{r}_{12} \\ &= \rho \int g\delta(\mathbf{r}_{12}) \left( \frac{1}{(2\pi)^3} \int \gamma(k) e^{ik \cdot r_{12}} d\mathbf{k} \right) d\mathbf{r}_{12} \\ &= \frac{\rho g}{(2\pi)^3} \int \gamma(k) d\mathbf{k}, \quad (\text{A3}) \\ & \frac{\rho}{2} \int V(r_{12}) \frac{2\rho}{(2\pi)^3} \left( \int \frac{\gamma^2(k)}{1-\rho\gamma(k)} e^{ik \cdot r_{12}} d\mathbf{k} \right) d\mathbf{r}_{12} \\ &= \frac{\rho^2}{(2\pi)^3} \int g\delta(\mathbf{r}_{12}) \left( \int \frac{\gamma^2(k)}{1-\rho\gamma(k)} e^{ik \cdot r_{12}} d\mathbf{k} \right) d\mathbf{r}_{12} \\ &= \frac{\rho^2 g}{(2\pi)^3} \int \frac{\gamma^2(k)}{1-\rho\gamma(k)} d\mathbf{k}. \quad (\text{A4}) \end{aligned}$$

We next consider the first term of Eq. (34). It vanishes, since  $f(r_{12})$  has no zero momentum components. Hence,

$$\frac{-\rho\hbar^2}{2m} \int \nabla^2 f(r_{12}) d\mathbf{r}_{12} = 0. \quad (\text{A5})$$

Considering the remaining terms of Eq. (34), we find

$$\begin{aligned} & \frac{-\rho\hbar^2}{2m} \int f(r_{12}) \nabla^2 f(r_{12}) d\mathbf{r}_{12} \\ &= \frac{-\rho\hbar^2}{2m} \int d\mathbf{r}_{12} \left( \frac{1}{(2\pi)^6} \int \gamma(k') e^{-ik' \cdot r_{12}} d\mathbf{k}' \right. \\ & \quad \left. \times \int -k^2 \gamma(k) e^{ik \cdot r_{12}} d\mathbf{k} \right) \\ &= \frac{\rho\hbar^2}{2m} \frac{1}{(2\pi)^3} \int k^2 \gamma^2(k) d\mathbf{k}, \quad (\text{A6}) \end{aligned}$$

$$\begin{aligned} & \frac{-\rho^3\hbar^2}{2m} \int d\mathbf{r}_{12} \nabla^2 f(r_{12}) \left( \frac{1}{(2\pi)^3} \int \frac{\gamma^3(k)}{1-\rho^2\gamma^2(k)} e^{ik \cdot r_{12}} d\mathbf{k} \right) \\ &= \frac{-\rho^3\hbar^2}{2m} \frac{1}{(2\pi)^6} \int d\mathbf{r}_{12} \left( \int -k'^2 \gamma(k') e^{-ik' \cdot r_{12}} d\mathbf{k}' \right. \\ & \quad \left. \times \int \frac{\gamma^3(k) e^{ik \cdot r_{12}}}{1-\rho^2\gamma^2(k)} d\mathbf{k} \right) \\ &= \frac{\rho^3\hbar^2}{2m} \frac{1}{(2\pi)^3} \int \frac{k^2 \gamma^4(k)}{1-\rho^2\gamma^2(k)} d\mathbf{k}. \quad (\text{A7}) \end{aligned}$$

Summing Eqs. (A2) through (A7) we obtain Eq. (36).