Ground State of a Bose System of Hard Spheres

TAI TSUN WU*
The Institute for Advanced Study, Princeton, New Jersey, and the Bell Telephone Laboratories, Murray Hill, New Jersey
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It is shown that the pseudopotential method can be extended to yield further terms in the low-density expansion of the ground-state energy of a system of Boltzmann or Bose particles with hard-sphere interaction. Two terms beyond the known result are found, and the expansion is no longer a power series in $(a^3\rho)^{\frac{1}{2}}$. Other related properties of the system are discussed.

1. INTRODUCTION

ALTHOUGH it is an old problem to investigate the properties of a system of a large number of particles interacting pairwise, there exists only a few explicit answers for the quantum mechanical case. In the case of a system of identical bosons interacting through the two-body hard-sphere potential, virtually none of its properties were known until the recent work of Yang, Lee, and Huang.[1–7] In the investigation of these authors, two independent methods have been used. One is the method of binary collision,[2,6,7] where the evaluation of the grand partition function is reduced to the solution of the two-body problem. In the other method,[1,3–5] use is made of the pseudopotential of Fermi. In both methods, the particle density is assumed to be low.

It is the aim of this paper to study the possibility of getting higher order terms by the method of the pseudopotential. One difficulty of the extension of this method is the inclusion of triple collision.[3] To the lowest order, this difficulty is resolved in Sec. 2. Another complication of the method of the pseudopotential, already apparent in reference 3, is the removal of the divergence in the expression for the ground-state energy per particle. This involves a comparision of the perturbation series with and without the operator $(\partial/\partial r)r$. This task becomes impossibly complicated in higher-order terms. In Sec. 3, a slight modification of the pseudopotential is proposed so that to the lowest order this removal of divergence is automatic. This is done at the expense of dealing with a non-Hermitian Hamiltonian at all times. In Sec. 4, this modified form of the pseudopotential is used to determine the next two terms in the expression for the ground-state energy per particle. However, in order to interpret the final formula, it is necessary to make a more detailed study of the three-body problem. This is done in Sec. 5, and the result is used in Sec. 6 to express the ground-state energy per particle for the many-particle system in a definitive form. In Sec. 7, some of the simple properties of the ground state are calculated. And finally Sec. 8 consists of some qualitative discussions of the present problem. This entire paper deals with the ground state only.

2. THREE-BODY PSEUDOPOTENTIAL

A system of hard spheres is a collection of pairwise interacting particles with the Hamiltonian ($\hbar=2m=1$)

$$H=T+V, \tag{2.1}$$

with

$$T=\sum_{i=1}^{N} p_i^2, \quad V=\sum_{i<j} V_0(r_{ij}), \tag{2.2}$$

where

$$r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|, \tag{2.3}$$

and

$$V_0(r)=\begin{cases} 0, & r>a \\ \infty, & r\leq a. \end{cases} \tag{2.4}$$

These particles are, as usual, assumed to be confined to a cubical box of volume $\Omega=L^3$, with periodic boundary conditions on its surface.

When $N=2$, the interaction potential may be replaced exactly by the pseudopotential[1]

$$V_2=\frac{8\pi \tan ka}{k}\delta(\mathbf{r}_1-\mathbf{r}_2)\frac{\partial}{\partial r_{12}}r_{12}+\text{terms corresponding to partial waves with } l\geq 1, \tag{2.5}$$

where the meaning of k has been discussed in reference 1. When applied to the case $N>2$, the replacement of V_0 by V_2 is accurate only when the interacting pair of particles are far away from all the other particles. Therefore, if V_0 is to be correctly represented by a pseudopotential, it is necessary to include a three-body pseudopotential in addition to V_2. To find this three-body pseudopotential, consider the case $N=3$. The problem is to find V_3 such that the eigenfunctions of

$$H_3=p_1^2+p_2^2+p_3^2+V_0(r_{23})+V_0(r_{31})+V_0(r_{12}) \tag{2.6}$$

and

$$H_3'=p_1^2+p_2^2+p_3^2+V_2(r_{23})+V_2(r_{31})+V_2(r_{12})+V_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \tag{2.7}$$

coincide in the region $r_{23}, r_{31}, r_{12}>a$.

* Junior Fellow, Society of Fellows, Harvard University. Now Assistant Professor of Applied Physics, Harvard University, Cambridge, Massachusetts.
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The pseudopotential V_2 as given by (2.5) is exceedingly complicated, but when

$$ka\ll 1, \tag{2.8}$$

the leading term is simply

$$V_2 \sim 8\pi a\delta(\mathbf{r}_1-\mathbf{r}_2)\frac{\partial}{\partial r_{12}}r_{12}. \tag{2.9}$$

In almost all applications of the pseudopotential, this approximation is used. In the same sense, the leading term of V_3 is, by dimensional arguments,[1]

$$V_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\sim \text{constant } a^4\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_2-\mathbf{r}_3)O_3, \tag{2.10}$$

where O_3 is some generalization of $(\partial/\partial r_{12})r_{12}$ to three bodies. It is the purpose of this section to find the constant in (2.10).

The meaning of the assumption (2.8) is that momenta comparable to or larger than a^{-1} are not important. In coordinate space, this means that distances comparable to or smaller than a are neglected. Therefore for the present purpose, the comparison of the two Hamiltonians in (2.6) and (2.7) may be carried out in the following manner. Instead of the eigenfunction problem originally posed, consider the scattering problem with the same Hamiltonian. In accordance with (2.8), the energy of the incident field is chosen to be small compared with a^{-2}. And the constant in (2.10) is to be so determined that the scattered fields for the two Hamiltonians coincide as well as possible for points far away from the region $\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}_3$. If the first Born approximation is used with respect to V_3, then the O_3 of (2.10) may be replaced by 1.

In order to carry out this program, the formalism of binary collision is used. Write (2.6) in the form

$$H_3=H_0+V_0^{23}+V_0^{31}+V_0^{12}, \tag{2.11}$$

and consider the Schrödinger equation

$$(H_3-E)\psi_0=0 \tag{2.12}$$

for a scattering problem. Let ψ^{inc} be the incident field satisfying $(H_0-E)\psi^{\text{inc}}=0$ and define the following operators:

$$G_0=-(H_0-E)^{-1}, \tag{2.13}$$

and

$$S_0^{23}=-(H_0+V_0^{23}-E)^{-1}V_0^{23}, \text{ etc.} \tag{2.14}$$

Note that the solution of

$$(H_0+V_0^{23}-E)\psi=0, \tag{2.15}$$

is

$$\psi=(1+S_0^{23})\psi^{\text{inc}}. \tag{2.16}$$

Equation (2.12) is equivalent to the integral equation

$$\psi_0=\psi^{\text{inc}}+G_0(V_0^{23}+V_0^{31}+V_0^{12})\psi_0. \tag{2.17}$$

But

$$G_0V_0^{23}=(1+S_0^{23})^{-1}S_0^{23}. \tag{2.18}$$

Thus the first two iterations of (2.17) give

$$\psi_0=(1+S_0^{23}+S_0^{31}+S_0^{12}+S_0^{31}S_0^{12}+S_0^{12}S_0^{23}+S_0^{23}S_0^{31} +S_0^{12}S_0^{31}+S_0^{23}S_0^{12}+S_0^{31}S_0^{23})\psi^{\text{inc}}. \tag{2.19}$$

It is required to compare ψ_0 with ψ_2, which is defined by the right-hand side of (2.19) with the subscript 0 replaced everywhere by 2. Here, for example,

$$S_2^{23}=-(H_0+V_2^{23}-E)^{-1}V_2^{23}. \tag{2.20}$$

From the way the pseudopotential V_2 is defined, it follows that

$$(S_0^{23}-S_2^{23})\psi^{\text{inc}}=0 \tag{2.21}$$

for $r_{23}>a$. Thus for the present purpose it is only necessary to study the quantity

$$D=D_1+D_2, \tag{2.22}$$

where

$$D_1=S_0^{12}(S_0^{23}-S_2^{23})\psi^{\text{inc}},$$

and

$$D_2=(S_0^{12}-S_2^{12})S_2^{23}\psi^{\text{inc}}. \tag{2.23}$$

In the determination of D_1, some properties of the following Green's function are needed:

$$(H_0-E)G=-\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_2-\mathbf{r}_3), \quad \mathbf{P}G=\mathbf{k}G, \tag{2.24}$$

where $\mathbf{P}$ is the total momentum and $k^2<3E$. Let

$$\mathbf{R}_3=\mathbf{r}_1+\mathbf{r}_2-2\mathbf{r}_3, \tag{2.25}$$

and

$$R^2=r_{23}{}^2+r_{31}{}^2+r_{12}{}^2=\tfrac{1}{2}(3r_{12}{}^2+R_3{}^2), \tag{2.26}$$

then a solution of (2.24) is

$$G=-i\frac{E_1\sqrt{3}}{48\pi^2}R^{-2}H_2^{(1)}(RE_1^{\frac{1}{2}}/\sqrt{3}) \times\exp[\tfrac{1}{3}i\mathbf{k}\cdot(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)], \tag{2.27}$$

where

$$E_1=E-\tfrac{1}{3}k^2. \tag{2.28}$$

The behavior of G for small R is

$$G=-\frac{\sqrt{3}}{4\pi^3}R^{-4}\exp[\tfrac{1}{3}i\mathbf{k}\cdot(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)]. \tag{2.29}$$

The equality $r_{12}=a$ defines a hypersurface in the six-dimensional space of relative coordinates $(\mathbf{r}_1-\mathbf{r}_2, \mathbf{R}_3)$. It follows from (2.29) that

$$\int_{r_{12}=a}Gd^5S=\int_{r_{12}=a}dS_{12}\int d^3\mathbf{R}_3\left(-\frac{\sqrt{3}}{4\pi^3}\right) \times 4(3r_{12}{}^2+R_3{}^2)^{-2}\exp[\tfrac{1}{3}i\mathbf{k}\cdot(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)] =-4a\exp[\tfrac{1}{3}i\mathbf{k}\cdot(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)]. \tag{2.30}$$

For the purpose of obtaining D_1, assume

$$\psi^{\text{inc}}=\exp[i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2+\mathbf{k}_3\cdot\mathbf{r}_3)], \tag{2.31}$$

with

$$k_1{}^2+k_2{}^2+k_3{}^2=E. \tag{2.32}$$

To first order, it follows from the definition of the pseudopotential that

$$(S_0^{23}-S_2^{23})\psi^{\text{inc}}=\left(\frac{a}{r_{23}}-1\right)h(a-r_{23})$$
$$\times\exp\{i[\mathbf{k}_1\cdot\mathbf{r}_1+\tfrac{1}{2}(\mathbf{k}_2+\mathbf{k}_3)\cdot(\mathbf{r}_2+\mathbf{r}_3)]\},\quad(2.33)$$

where h is the Heaviside function defined by

$$h(x)=1\quad\text{for}\quad x\geq 0$$
$$=0\quad\text{for}\quad x<0.\quad(2.34)$$

Therefore, for $r_{12}>a$, D_1 is a solution of

$$(H_0-E)D_1=0\quad(2.35)$$

with the boundary condition that, for $r_{12}=a$, $-D_1$ is equal to the right-hand side of (2.33). With

$$\mathbf{k}=\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3,\quad(2.36)$$

the right-hand side of (2.33) is approximately, for $r_{12}=a$,

$$\left(\frac{a}{r_{23}}-1\right)h(a-r_{23})\exp[\tfrac{1}{3}i\mathbf{k}\cdot(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)].\quad(2.37)$$

In particular, for fixed $\mathbf{r}_1-\mathbf{r}_2$,

$$\int d^3\mathbf{R}_3\left(\frac{a}{r_{23}}-1\right)h(a-r_{23})$$
$$=32\pi\int^{\infty} r_{23}{}^2dr_{23}\left(\frac{a}{r_{23}}-1\right)h(a-r_{23})=(16\pi/3)a^3,\quad(2.38)$$

which is independent of $\mathbf{r}_1-\mathbf{r}_2$. A comparison of (2.38) with (2.30) gives the result that

$$D_1=-(16/3)\pi^2a^4G.\quad(2.39)$$

The quantity D_2 may be calculated as follows. First it follows from (2.20) that

$$S_2^{23}\psi^{\text{inc}}=8\pi aG_0\delta(\mathbf{r}_2-\mathbf{r}_3).\quad(2.40)$$

For a point source in $r_{12}>a$, $S_0^{12}-S_2^{12}$ gives 0. For a point source in $r_{12}<a$, S_0^{12} may be replaced by -1, while S_2^{12} may be replaced by $-a/r_{12}$. Therefore

$$D_2/G=\tfrac{1}{8}\int d^3(\mathbf{r}_1-\mathbf{r}_2)d^3\mathbf{R}_3 8\pi a\delta(\mathbf{r}_2-\mathbf{r}_3)$$
$$\times\left(-1+\frac{a}{r_{12}}\right)h(a-r_{12})=(16\pi^2/3)a^4.\quad(2.41)$$

Finally, the substitution of (2.39) and (2.41) into (2.22) yields

$$D=0.\quad(2.42)$$

This means that for the purpose of the present calculation, there is no difference between ψ_0 and ψ_2. Since this result is independent of E.

$$V_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=0.\quad(2.43)$$

This means that the constant of (2.10) is zero, and consequently it is irrelevant what O_3 is.

In particular, there is no correction to the ground-state energy due to the three-body pseudopotential, to the order ρ^2a^4N, where $\rho=N/\Omega$ is the particle density.

3. TWO-BODY PSEUDOPOTENTIAL

Even in the case $N=2$, the pseudopotential $8\pi a\delta(\mathbf{r}_1-\mathbf{r}_2)(\partial/\partial r_{12})r_{12}$ of (2.9) cannot be replaced by $8\pi a\delta(\mathbf{r}_1-\mathbf{r}_2)$. However, in the treatment of the N-body system with large N, this replacement is made,[3,4] and leads to a divergence in, for example, the expression for the ground-state energy per particle. The removal of this divergence is a rather complicated process. This difficulty stems from the fact that the operator

$$O=\delta(\mathbf{r})\frac{\partial}{\partial r}r=\delta(\mathbf{r})\left[\frac{\partial}{\partial r}r\right]_{r=0}\quad(3.1)$$

does not commute with the infinite Fourier series; for example:

$$O\sum_{m\neq n}\frac{m\sin mr}{m^2-n^2}\neq\sum_{m\neq n}O\frac{m\sin mr}{m^2-n^2}.\quad(3.2)$$

This inequality causes trouble because a typical ψ for O to operate on is a solution of

$$(\nabla^2+k^2)\psi=4\pi ka\delta(\mathbf{r}).\quad(3.3)$$

It is the purpose of this section to see how the operator O can be slightly modified so that this particular divergence does not occur. The modified form of the pseudopotential is then used to get the phonon spectrum near the ground state and the ground-state energy.

Imagine that the $\delta(\mathbf{r})$ in (3.1) is replaced by, for example,

$$\delta_{\epsilon'}(\mathbf{r})=(8\pi\epsilon'^3)^{-1}e^{-r/\epsilon'},\quad(3.4)$$

where $\epsilon'\ll a$. To be consistant, the $\delta(\mathbf{r})$ in (3.3) has to be so replaced also. In this case, ψ is distorted up to a distance several times ϵ'. In order that the pseudopotential can serve its purpose, the part $(\partial/\partial r)r$ of (3.1) should be evaluated at a distance ϵ, where $\epsilon'\ll\epsilon\ll a$. Since only an S wave is under consideration, the result is more precisely

$$O_{\epsilon\epsilon'}=\delta_{\epsilon'}(\mathbf{r})\left[\frac{1}{4\pi}\int d\Omega\frac{\partial}{\partial r}r\right]_{r=\epsilon}.\quad(3.5)$$

Since ϵ' is much smaller than any other length in the problem, it may be set to zero. Then (3.5) becomes

$$O_\epsilon=\delta(\mathbf{r})\left[\frac{1}{4\pi}\int d\Omega\frac{\partial}{\partial r}r\right]_{r=\epsilon}.\quad(3.6)$$

For a ψ with no singularity at $r=\epsilon$, O_ϵ commutes with the Fourier decomposition; for example, in contrast to (3.2),

$$O_\epsilon\sum_{m\neq n}\frac{m\sin mr}{m^2-n^2}=\sum_{m\neq n}O_\epsilon\frac{m\sin mr}{m^2-n^2}.\quad(3.7)$$

It is proposed here to use the O_ϵ of (3.6) in the two-body pseudopotential instead of O. Only after the desired answers are obtained will the limit $\epsilon \to 0+$ be taken. More precisely, the order of the limits are $\lim_{\epsilon\to 0+} \lim_{\Omega\to\infty}$, where the right-hand limit means $N \to \infty$ so that $\rho = N/\Omega$ is fixed.

It may be noted that

$$O_\epsilon^2 = 0. \quad (3.8)$$

With the result of Sec. 2 and this interpretation of the pseudopotential (2.9), the Hamiltonian of a Bose system of hard spheres may be approximated by

$$H' = T + V'. \quad (3.9)$$

with

$$T = -\int d^3\mathbf{r}\psi^*(\mathbf{r})\nabla^2\psi(\mathbf{r}), \quad (3.10)$$

and

$$V' = a\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \psi^*(\mathbf{r}_1)\psi^*(\mathbf{r}_2)\delta(\mathbf{r}_1-\mathbf{r}_2) \times\left[\int d\Omega_{12}\frac{\partial}{\partial r_{12}} r_{12}\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\right]_{r_{12}=\epsilon}. \quad (3.11)$$

Here the language of quantized fields is used, and ψ satisfies the usual commutation rules for a boson field. In (3.11), $\partial/\partial r_{12}$ is taken with fixed $\mathbf{r}_1+\mathbf{r}_2$. If the annihilation operators in the momentum space are defined by

$$\psi(\mathbf{r}) = \Omega^{-\frac{1}{2}} \sum_\mu a_\mu \exp(i\mathbf{k}_\mu\cdot\mathbf{r}), \quad (3.12)$$

then

$$T = \sum_\mu k_\mu^2 a_\mu^* a_\mu, \quad (3.13)$$

and

$$V' = \Omega^{-1}4\pi a \sum_{\alpha,\beta,\mu,\nu} a_\alpha^* a_\beta^* a_\mu a_\nu \delta(\mathbf{k}_\alpha+\mathbf{k}_\beta-\mathbf{k}_\mu-\mathbf{k}_\nu) \times\cos(\tfrac{1}{2}\epsilon|\mathbf{k}_\mu-\mathbf{k}_\nu|). \quad (3.14)$$

This differs from the V' of Lee, Huang, and Yang[3] only in the appearance of the cosine factor. When the occupation of the $k=0$ state is almost complete, and only pair excitation is included, an approximate formula for V' is

$$V' = 4\pi a\rho N + 4\pi a\rho \sum_{\mathbf{k}\neq 0} [a_\mathbf{k}^* a_\mathbf{k}(4\cos\tfrac{1}{2}\epsilon k - 2) + a_\mathbf{k}^* a_{-\mathbf{k}}^* + a_\mathbf{k} a_{-\mathbf{k}} \cos\epsilon k]. \quad (3.15)$$

If the following notations are used,

$$k_0^2 = 8\pi a\rho, \quad (3.16)$$

$$y_k = \tfrac{1}{2}k_0^2[k^2+k_0^2(2\cos\tfrac{1}{2}\epsilon k - 1)]^{-1}, \quad (3.17)$$

then

$$H' = 4\pi a\rho N + \sum_{\mathbf{k}\neq 0} [k^2+k_0^2(2\cos\tfrac{1}{2}\epsilon k-1)] \times[a_\mathbf{k}^* a_\mathbf{k} + y_k(a_\mathbf{k}^* a_{-\mathbf{k}}^* + a_\mathbf{k} a_{-\mathbf{k}}\cos\epsilon k)]. \quad (3.18)$$

The eigenvalues of this non-Hermitian Hamiltonian give the energies of the low-lying states of the Bose system.

In view of the form of the Hamiltonian of (3.18), let

$$H_\mathbf{k} = a_\mathbf{k}^* a_\mathbf{k} + a_{-\mathbf{k}}^* a_{-\mathbf{k}} + 2y_k(a_\mathbf{k}^* a_{-\mathbf{k}}^* + a_\mathbf{k} a_{-\mathbf{k}} \cos\epsilon k), \quad (3.19)$$

where $\mathbf{k}\neq 0$. This Hamiltonian, being non-Hermitian, cannot be diagonalized by a canonical transformation of the form[8]

$$\xi_\mathbf{k} = (1-\alpha_k^2)^{-\frac{1}{2}}(a_\mathbf{k} + \alpha_k a_{-\mathbf{k}}^*),$$
$$\xi_{-\mathbf{k}} = (1-\alpha_k^2)^{-\frac{1}{2}}(a_{-\mathbf{k}} + \alpha_k a_\mathbf{k}^*). \quad (3.20)$$

However, if α_k is chosen to be

$$\alpha_k = (2y_k\cos\epsilon k)^{-1}[1-(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}], \quad (3.21)$$

then

$$H_\mathbf{k} = -[1-(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}] + (1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}(\xi_\mathbf{k}^*\xi_\mathbf{k} + \xi_{-\mathbf{k}}^*\xi_{-\mathbf{k}}) - 2y_k(1-\cos\epsilon k)\xi_\mathbf{k}\xi_{-\mathbf{k}}. \quad (3.22)$$

On the other hand, if the choice is

$$\bar{\alpha}_k = (2y_k)^{-1}[1-(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}], \quad (3.23)$$

then

$$H_\mathbf{k} = -[1-(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}] + (1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}(\bar{\xi}_\mathbf{k}^*\bar{\xi}_\mathbf{k} + \bar{\xi}_{-\mathbf{k}}^*\bar{\xi}_{-\mathbf{k}}) + 2y_k(1-\cos\epsilon k)\bar{\xi}_\mathbf{k}^*\bar{\xi}_{-\mathbf{k}}^*. \quad (3.24)$$

Since $\xi_\mathbf{k}$ and $\bar{\xi}_\mathbf{k}$ separately satisfy the same commutation rules as $a_\mathbf{k}$, it follows from either (3.22) or (3.24) that the energy eigenvalues of $H_\mathbf{k}$ are

$$E_\mathbf{k}(m_\mathbf{k}, m_{-\mathbf{k}}) = -[1-(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}] + (m_\mathbf{k}+m_{-\mathbf{k}})(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}. \quad (3.25)$$

The substitution into (3.18) then yields the phonon spectrum near the ground state

$$E(m_\mathbf{k}) = E_0 + E_{\text{phonon}}(m_\mathbf{k}), \quad (3.26)$$

where

$$E_0 = 4\pi a\rho N + \tfrac{1}{2}\sum_{\mathbf{k}\neq 0}[k^2+k_0^2(2\cos\tfrac{1}{2}\epsilon k-1)] \times[-1+(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}], \quad (3.27)$$

and

$$E_{\text{phonon}}(m_\mathbf{k}) = \sum_{\mathbf{k}\neq 0} m_\mathbf{k}[k^2+k_0^2(2\cos\tfrac{1}{2}\epsilon k-1)] \times(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}. \quad (3.28)$$

Equation (3.26) is valid when $m_\mathbf{k} = O(1)$, and $\sum_{\mathbf{k}\neq 0} m_\mathbf{k} = o(N)$. In the limit $\epsilon \to 0+$, (3.28) yields the well-known formula[3,4]

$$E_{\text{phonon}}(m_\mathbf{k}) = \sum_{\mathbf{k}\neq 0} m_\mathbf{k} k(k^2+16\pi a\rho)^{\frac{1}{2}}. \quad (3.29)$$

In the same limit, (3.27) yields the ground-state energy per particle

[8] N. N. Bogoliubov, J. Phys. (U.S.S.R.) **11**, 23 (1947).

$$E_0/N=4\pi a\rho+\lim_{\epsilon\to 0+}\lim_{\Omega\to\infty}(2\rho\Omega)^{-1}\times\sum_{\mathbf{k}\neq 0}[k^2+k_0^2(2\cos\tfrac{1}{2}\epsilon k-1)]\times[-1+(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}]$$
$$=4\pi a\rho+\lim_{\epsilon\to 0+}(4\pi^2\rho)^{-1}\times\int_0^\infty dk k^2[k^2+k_0^2(2\cos\tfrac{1}{2}\epsilon k-1)]\times[-1+(1-4y_k^2\cos\epsilon k)^{\frac{1}{2}}]. \quad (3.30)$$

As $k\to\infty$, the integrand is asymptotically $-\frac{1}{2}k_0^4\cos\epsilon k$, which yields zero when integrated from 0 to ∞ for any $\epsilon\neq 0$. If this asymptotic expression is subtracted from the integrand, the limit $\epsilon\to 0+$ may be taken under the integral sign to give the result

$$E_0/N=4\pi a\rho+(4\pi^2\rho)^{-1}\int_0^\infty dk\{k^2(k^2+k_0^2)\times[-1+(1-4y_k^2|_{\epsilon=0})^{\frac{1}{2}}]+\tfrac{1}{2}k_0^4\}. \quad (3.31)$$

This is identical with the result of Lee, Huang, and Yang.[2,3] After integration, the result is

$$E_0/N=4\pi a\rho\left[1+\frac{128}{15\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}}\right]. \quad (3.32)$$

The present procedure involves no removal of divergence. Note also that in this calculation the combination $2\cos\frac{1}{2}\epsilon k-1$ in (3.17) and (3.18) may be replaced by 1 at the beginning.

Now consider the lowest state of $H_{\mathbf{k}}$. Since it is necessary to distinguish the right and left states, define $\langle 0_{\mathbf{k}}|$ and $|0_{\mathbf{k}}\rangle$ by

$$\xi_{\mathbf{k}}|0_{\mathbf{k}}\rangle=\xi_{-\mathbf{k}}|0_{\mathbf{k}}\rangle=0,\quad \langle 0_{\mathbf{k}}|\bar{\xi}_{\mathbf{k}}^*=\langle 0_{\mathbf{k}}|\bar{\xi}_{-\mathbf{k}}^*=0. \quad (3.33)$$

In terms of $a_{\mathbf{k}}$, (3.33) is, with (3.20),

$$(a_{\mathbf{k}}+\alpha_k a_{-\mathbf{k}}^*)|0_{\mathbf{k}}\rangle=(a_{-\mathbf{k}}+\alpha_k a_{\mathbf{k}}^*)|0_{\mathbf{k}}\rangle=0,\quad \langle 0_{\mathbf{k}}|(a_{\mathbf{k}}^*+\bar{\alpha}_k a_{-\mathbf{k}})=\langle 0_{\mathbf{k}}|(a_{-\mathbf{k}}^*+\bar{\alpha}_k a_{\mathbf{k}})=0. \quad (3.34)$$

From (3.34), except for normalizations, the states $|0_{\mathbf{k}}\rangle$ and $\langle 0_{\mathbf{k}}|$ may be expressed in terms of the states $|\,\rangle$ and $\langle\,|$ defined by

$$a_{\mathbf{k}}|\,\rangle=0,\quad \langle\,|a_{\mathbf{k}}^*=0. \quad (3.35)$$

The results are

$$|0_{\mathbf{k}}\rangle=K_k\exp(-\alpha_k a_{\mathbf{k}}^*a_{-\mathbf{k}}^*)|\,\rangle,\quad \langle 0_{\mathbf{k}}|=\bar{K}_k\langle\,|\exp(-\bar{\alpha}_k a_{\mathbf{k}}a_{-\mathbf{k}}). \quad (3.36)$$

The normalization

$$\langle 0_{\mathbf{k}}|0_{\mathbf{k}}\rangle=1 \quad (3.37)$$

then yields the condition

$$K_k\bar{K}_k=1-\alpha_k\bar{\alpha}_k. \quad (3.38)$$

The state of $H_{\mathbf{k}}$ with one phonon of momentum $\mathbf{k}$ is related to the lowest state by

$$|1_{\mathbf{k}}\rangle=K_k'\xi_{\mathbf{k}}^*|0_{\mathbf{k}}\rangle,\quad \langle 1_{\mathbf{k}}|=\bar{K}_k'\langle 0_{\mathbf{k}}|\bar{\xi}_{\mathbf{k}}. \quad (3.39)$$

Since

$$\langle 0_{\mathbf{k}}|a_{\mathbf{k}}a_{-\mathbf{k}}|0_{\mathbf{k}}\rangle=-\alpha_k(1-\alpha_k\bar{\alpha}_k)^{-1},$$
$$\langle 0_{\mathbf{k}}|a_{\mathbf{k}}^*a_{-\mathbf{k}}^*|0_{\mathbf{k}}\rangle=-\bar{\alpha}_k(1-\alpha_k\bar{\alpha}_k)^{-1},$$
$$\langle 0_{\mathbf{k}}|a_{\mathbf{k}}^*a_{\mathbf{k}}|0_{\mathbf{k}}\rangle=\langle 0_{\mathbf{k}}|a_{-\mathbf{k}}^*a_{-\mathbf{k}}|0_{\mathbf{k}}\rangle=\alpha_k\bar{\alpha}_k(1-\alpha_k\bar{\alpha}_k)^{-1}, \quad (3.40)$$

as consequences of (3.36) and (3.38), the normalization

$$\langle 1_{\mathbf{k}}|1_{\mathbf{k}}\rangle=1 \quad (3.41)$$

yields the condition

$$K_k'\bar{K}_k'=(1-\alpha_k^2)^{-\frac{1}{2}}(1-\bar{\alpha}_k^2)^{-\frac{1}{2}}(1-\alpha_k\bar{\alpha}_k). \quad (3.42)$$

The states $|m_{\mathbf{k}},m_{-\mathbf{k}}\rangle$ with both numbers different from zero are somewhat more complicated, although explicit formulas can be found for them. They do not appear in the following discussion. It may be noted that, as a consequence of the pair excitation, it is possible to choose the normalization

$$\langle m_{\mathbf{k}},m_{-\mathbf{k}}|m_{\mathbf{k}}',m_{-\mathbf{k}}'\rangle=\delta_{m_{\mathbf{k}},m_{\mathbf{k}}'}\delta_{m_{-\mathbf{k}},m_{-\mathbf{k}}'} \quad (3.43)$$

even though $H_{\mathbf{k}}$ is not Hermitian.

4. GROUND-STATE ENERGY PER PARTICLE

It is the purpose of this section to improve the calculation of the previous section for the ground-state energy per particle by applying the second-order perturbation theory after the canonical transformation. For this purpose, attention is returned to (3.13) and (3.14). A more accurate approximation of V' than (3.15) may be obtained as follows.

A. Let $n_0=\langle a_0^*a_0\rangle$, where the expectation value is taken in the ground state; then

$$a_0^*a_0^*a_0a_0\sim(a_0^*a_0)^2=[n_0+(a_0^*a_0-n_0)]^2\sim n_0^2+2n_0(a_0^*a_0-n_0)=n_0(2N-n_0)-2n_0\sum_{\mathbf{k}\neq 0}a_{\mathbf{k}}^*a_{\mathbf{k}}. \quad (4.1)$$

Here, use has been made of the relation $N=\sum_{\mathbf{k}}a_{\mathbf{k}}^*a_{\mathbf{k}}$.

B. In view of the remark following (3.32), ϵ may be made equal to 0 in those terms of V' that can be combined directly with kinetic energy terms. Thus

$$a_0^*a_{\mathbf{k}}^*a_0a_{\mathbf{k}}\cos\tfrac{1}{2}k\epsilon\sim a_0^*a_{\mathbf{k}}^*a_0a_{\mathbf{k}}\sim n_0a_{\mathbf{k}}^*a_{\mathbf{k}} \quad (4.2)$$

for $\mathbf{k}\neq 0$.

C. The same approximation may also be used in the numerical part of the Hamiltonian. Thus

$$\sum_{\alpha,\beta\neq 0}a_\alpha^*a_\beta^*a_\alpha a_\beta\cos(\tfrac{1}{2}\epsilon|\mathbf{k}_\alpha-\mathbf{k}_\beta|)\sim\sum_{\alpha,\beta\neq 0}a_\alpha^*a_\beta^*a_\alpha a_\beta\sim(N-a_0^*a_0)^2\sim(N-n_0)^2. \quad (4.3)$$

D. For the off-diagonal terms, the approximation

$$a_0 \sim a_0^* \sim n_0^{\frac{1}{2}} \tag{4.4}$$

may be used.

E. For the off-diagonal terms, those with four momenta all different from zero are neglected.

These approximations are based on the fact that $1-n_0/N$ is small; more precisely, Lee, Huang, and Yang[9] have given the result

$$\xi = n_0/N = 1 - \frac{8}{3\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}} + o[(a^3\rho)^{\frac{1}{2}}]. \tag{4.5}$$

This quantity is to be studied in more detail in Sec. 7.

It is convenient at this stage to modify (3.16) to

$$k_0^2 = 8\pi a\rho\xi, \tag{4.6}$$

and, according to (4.2), to simplify (3.17) to read

$$y_k = \tfrac{1}{2}k_0^2(k^2+k_0^2)^{-1}. \tag{4.7}$$

With these notations and the approximations $A-E$, the Hamiltonian given by (3.9), (3.13), and (3.14) becomes

$$\begin{aligned} H' &= 4\pi a\rho N[1+(1-\xi)^2] + \sum_{\mathbf{k}\neq 0}(k^2+k_0^2) \\ &\quad \times [a_{\mathbf{k}}^* a_{\mathbf{k}} + y_k(a_{\mathbf{k}}^* a_{-\mathbf{k}}^* + a_{\mathbf{k}} a_{-\mathbf{k}} \cos k\epsilon)] \\ &\quad + \Omega^{-1} 8\pi a n_0^{\frac{1}{2}} \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}+\mathbf{k}'\neq 0} [a_{\mathbf{k}}^* a_{\mathbf{k}'}^* a_{\mathbf{k}+\mathbf{k}'} \cos(\tfrac{1}{2}|\mathbf{k}+\mathbf{k}'|\epsilon) \\ &\quad + a_{\mathbf{k}+\mathbf{k}'}^* a_{\mathbf{k}} a_{\mathbf{k}'} \cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|\epsilon)] \\ &\quad + \Omega^{-1} 4\pi a \sum_{\mathbf{k},\mathbf{k}'\neq 0} a_{\mathbf{k}}^* a_{-\mathbf{k}}^* a_{\mathbf{k}'} a_{-\mathbf{k}'} \cos k'\epsilon. \end{aligned} \tag{4.8}$$

The first two terms of this Hamiltonian are identical in form with the Hamiltonian of (3.18). Therefore, with some trivial modifications, the canonical transformations of last section may also be applied to the present case. The program is to treat these two terms as the unperturbed Hamiltonian and then carry out a second-order perturbation calculation to get the ground-state energy per particle. For this purpose, certain matrix elements have to be obtained.

With reference to (3.33), the right and left unperturbed ground states may be defined by

$$\begin{aligned} \xi_{\mathbf{k}}|0\rangle &= 0, \\ \langle 0|\bar{\xi}_{\mathbf{k}} &= 0, \end{aligned} \tag{4.9}$$

for all $\mathbf{k}\neq 0$, where $\xi_{\mathbf{k}}$ and $\bar{\xi}_{\mathbf{k}}$ are defined by (3.20), (3.21), and (3.23) with the y_k of (4.7) and (4.6). In view of the form of (4.8), one matrix element to be calculated is

$$\Delta E_1 = \langle 0|\Omega^{-1}4\pi a \sum_{\mathbf{k},\mathbf{k}'\neq 0} a_{\mathbf{k}}^* a_{-\mathbf{k}}^* a_{\mathbf{k}'} a_{-\mathbf{k}'} \cos k'\epsilon|0\rangle. \tag{4.10}$$

This may be evaluated using $|0_{\mathbf{k}}\rangle$ and the identities (3.40) as follows:

$$\begin{aligned} \Delta E_1 &= \Omega^{-1}4\pi a[\sum_{\mathbf{k}\neq 0}\langle 0_{\mathbf{k}}|a_{\mathbf{k}}^* a_{-\mathbf{k}}^*|0_{\mathbf{k}}\rangle] \\ &\quad \times [\sum_{\mathbf{k}'\neq 0}\langle 0_{\mathbf{k}'}|a_{\mathbf{k}'} a_{-\mathbf{k}'}|0_{\mathbf{k}'}\rangle \cos k'\epsilon] \\ &= \Omega^{-1}4\pi a[\sum_{\mathbf{k}\neq 0}\bar{\alpha}_k(1-\alpha_k\bar{\alpha}_k)^{-1}] \\ &\quad \times [\sum_{\mathbf{k}\neq 0}\alpha_k(1-\alpha_k\bar{\alpha}_k)^{-1}\cos k\epsilon]. \end{aligned} \tag{4.11}$$

This is easily evaluated in the limit $\Omega\to\infty$ and then $\epsilon\to 0+$:

$$\Delta E_1/N = 4\pi a\rho(64a^3\rho/\pi). \tag{4.12}$$

Accordingly, the diagonal matrix element of the H' of (4.8) is

$$\langle 0|H'|0\rangle = 4\pi a\rho N\left[1+(1-\xi)^2 + \frac{128}{15}\xi^{\frac{5}{2}}\left(\frac{a^3\rho}{\pi}\right)^{\frac{1}{2}} + 64\xi^3\left(\frac{a^3\rho}{\pi}\right)\right]. \tag{4.13}$$

When (4.5) is substituted in (4.13), the result is more explicitly

$$\langle 0|H'|0\rangle = 4\pi a\rho N\left[1+\frac{128}{15}\left(\frac{a^3\rho}{\pi}\right)^{\frac{1}{2}} + \frac{128}{9}\left(\frac{a^3\rho}{\pi}\right)\right]. \tag{4.14}$$

It is seen from (4.8) that the relevant intermediate states for a second-order perturbation calculation are the three-phonon states. In view of (3.39), they may be defined by

$$\begin{aligned} |1_{\mathbf{k}},1_{\mathbf{k}'},1_{\mathbf{k}''}\rangle &= K_k' K_{k'}' K_{k''}' \xi_{\mathbf{k}}^* \xi_{\mathbf{k}'}^* \xi_{\mathbf{k}''}^* |0\rangle, \\ \langle 1_{\mathbf{k}},1_{\mathbf{k}'},1_{\mathbf{k}''}| &= \bar{K}_k' \bar{K}_{k'}' \bar{K}_{k''}' \langle 0|\bar{\xi}_{\mathbf{k}}\bar{\xi}_{\mathbf{k}'}\bar{\xi}_{\mathbf{k}''}, \end{aligned} \tag{4.15}$$

where the three $\mathbf{k}$'s are assumed to be distinct. With the help of (3.20) and (3.40), it is not difficult to verify that for $\mathbf{k}+\mathbf{k}'+\mathbf{k}''=0$

$$\begin{aligned} \langle 1_{\mathbf{k}},1_{\mathbf{k}'},1_{\mathbf{k}''}|H'|0\rangle &= \Omega^{-1}16\pi a n_0^{\frac{1}{2}} \bar{K}_k' \bar{K}_{k'}' \bar{K}_{k''}' (1-\bar{\alpha}_k^2)^{\frac{1}{2}} \\ &\quad \times (1-\bar{\alpha}_{k'}^2)^{\frac{1}{2}}(1-\bar{\alpha}_{k''}^2)^{\frac{1}{2}}(1-\alpha_k\bar{\alpha}_k)^{-1}(1-\alpha_{k'}\bar{\alpha}_{k'})^{-1} \\ &\quad \times (1-\alpha_{k''}\bar{\alpha}_{k''})^{-1}[-\alpha_{k''}\cos(\tfrac{1}{2}k''\epsilon) \\ &\qquad + \alpha_k\alpha_{k'}\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|\epsilon) + \text{symm.}], \end{aligned}$$

and (4.16)

$$\begin{aligned} \langle 0|H'|1_{\mathbf{k}},1_{\mathbf{k}'},1_{\mathbf{k}''}\rangle &= \Omega^{-1}16\pi a n_0^{\frac{1}{2}} K_k' K_{k'}' K_{k''}' (1-\alpha_k^2)^{\frac{1}{2}} \\ &\quad \times (1-\alpha_{k'}^2)^{\frac{1}{2}}(1-\alpha_{k''}^2)^{\frac{1}{2}}(1-\alpha_k\bar{\alpha}_k)^{-1}(1-\alpha_{k'}\bar{\alpha}_{k'})^{-1} \\ &\quad \times (1-\alpha_{k''}\bar{\alpha}_{k''})^{-1}[\bar{\alpha}_k\bar{\alpha}_{k'}\cos(\tfrac{1}{2}k''\epsilon) \\ &\qquad - \bar{\alpha}_{k''}\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|\epsilon) + \text{symm.}], \end{aligned} \tag{4.17}$$

where "symm." denotes additional terms obtained from those explicitly written down by the cyclic permutations of the three indices. So far as the energy denominator is concerned, it is sufficient to use the phonon spectrum (3.29). With (3.42), the ground-state energy shift due to the three-phonon processes is found to be

[9] See Eq. (40b) of reference 3. There the α should be a.

$$\Delta E_2 = -\sum_{\substack{k>k'>k''>0 \\ \mathbf{k}+\mathbf{k}'+\mathbf{k}''=0}} (E_k+E_{k'}+E_{k''})^{-1} 256\pi^2 a^2 \rho \Omega^{-1}$$
$$\times (1-\alpha_k\bar{\alpha}_k)^{-1}(1-\alpha_{k'}\bar{\alpha}_{k'})^{-1}(1-\alpha_{k''}\bar{\alpha}_{k''})^{-1}$$
$$\times [\bar{\alpha}_k\bar{\alpha}_{k'}\cos(\tfrac{1}{2}k''\epsilon)-\bar{\alpha}_{k''}\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|\epsilon)+\text{symm.}]$$
$$\times [-\alpha_{k''}\cos(\tfrac{1}{2}k''\epsilon)+\alpha_k\alpha_{k'}\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|\epsilon)+\text{symm.}], \quad (4.18)$$

where

$$E_k = k(k^2+16\pi a\rho)^{\frac{1}{2}}. \quad (4.19)$$

In (4.18) the approximation $\xi=1$ may be used. Unfortunately, as it stands, the formula (4.18) is not meaningful, because $\lim_{\epsilon\to 0+}\lim_{\Omega\to\infty}\Delta E_2$ does not exist. This difficulty is to be resolved in the next two sections.

5. THE THREE-BODY PROBLEM

The difficulty with (4.18) is not peculiar to the N-body problem for large N, in the sense that a very similar trouble already appears in the three-body problem. Rather, this difficulty may be considered to be a fundamental limitation of the method of the pseudopotential. This section is devoted to a study of the ground-state energy of a system of three particles interacting pairwise through the hard-sphere potential V_0 and confined to a large periodic cubic box of volume Ω.

This limitation of the pseudopotential of (2.9) may be seen from the perturbation calculation of the N-body ground-state energy by Huang and Yang.[1] There, the energy is calculated to the third order. If one attempts to carry the procedure further to get the fourth-order energy, the result is divergent for $N>2$. The divergence is unrelated to the one arising from the omission of the operator $(\partial/\partial r)r$. Furthermore, the situation here is not improved by the introduction of ϵ: the fourth-order energy is convergent for $\epsilon>0$, but as $\epsilon\to 0+$, the limit does not exist. Since this fourth-order energy is useful in spite of this difficulty, this perturbation calculation is repeated here with ϵ. Only the case $N=3$ is treated since further generalization does not seem to be necessary.

Consider the three-body Hamiltonian

$$H_3' = p_1^2+p_2^2+p_3^2+H_1, \quad (5.1)$$

with

$$H_1 = 8\pi a\left\{\delta(\mathbf{r}_2-\mathbf{r}_3)\left[\frac{1}{4\pi}\int d\Omega_{23}\frac{\partial}{\partial r_{23}}r_{23}\right]_{r_{23}=\epsilon}+\text{symm.}\right\}, \quad (5.2)$$

where "symm." again denotes the other two terms obtained from the first one by the cyclic permutation of the indices 1, 2, 3. The three particles are confined in a cubical box of sizes $L\times L\times L$ with periodic boundary conditions. It is assumed that

$$\epsilon \ll a \ll L. \quad (5.3)$$

For the perturbation calculation of the ground-state energy, the three particles may be assumed to be distinguishable. Then the eigenstates of the kinetic energy part of the Hamiltonian (5.1) are the momentum states $|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle$ with the coordinate representation

$$\langle \mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle = \Omega^{-\frac{3}{2}}\exp[i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2+\mathbf{k}_3\cdot\mathbf{r}_3)]. \quad (5.4)$$

In terms of these momentum states, the matrix elements of H_1 of (5.2) are

$$\langle \mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3'|H_1|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle = \Omega^{-1}8\pi a[\delta_{\mathbf{k}_1\mathbf{k}_1'}\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon)+\text{symm.}]. \quad (5.5)$$

The first three orders of perturbation yield just the following results by Huang and Yang,[1] in the limit $\epsilon\to 0$:

$$E^{(1)} = 24\pi a/\Omega,$$
$$E^{(2)} = C(a/L)E^{(1)}, \quad (5.6)$$
$$E^{(3)} = (C^2+\xi_2)(a/L)^2E^{(1)},$$

where C is a constant approximately equal to 2.37 and ξ_α with $\alpha\geq 2$ is defined by

$$\xi_\alpha = \pi^{-\alpha}\sum_{l,m,n=-\infty}^{\infty}{}' (l^2+m^2+n^2)^{-\alpha}. \quad (5.7)$$

This perturbation calculation is now to be pushed to fourth order. Let G_0 be the operator defined by (2.13) with $E=0$:

$$G_0 = -(p_1^2+p_2^2+p_3^2)^{-1}, \quad (5.8)$$

and Q be the projection operator

$$Q = 1-|\mathbf{0},\mathbf{0},\mathbf{0}\rangle\langle\mathbf{0},\mathbf{0},\mathbf{0}|. \quad (5.9)$$

Then $E^{(4)}$ consists of two parts, one of which can be easily obtained in the limit $\epsilon\to 0+$:

$$E^{(4)} = E_1^{(4)}+E_2^{(4)}, \quad (5.10)$$

where

$$E_1^{(4)} = (-9C\xi_2+15\xi_3)(a/L)^3E^{(1)} \quad (5.11)$$

in the limit $\epsilon\to 0+$, and

$$E_2^{(4)} = \langle\mathbf{0},\mathbf{0},\mathbf{0}|H_1G_0QH_1G_0QH_1G_0QH_1|\mathbf{0},\mathbf{0},\mathbf{0}\rangle. \quad (5.12)$$

With (5.5) the right-hand side of (5.12) may be found explicitly. It again consists of two parts, one of them being in a form not dissimilar to $E_1^{(4)}$:

$$E_2^{(4)} = E_3^{(4)}+E_4^{(4)}, \quad (5.13)$$

where

$$E_1^{(4)}+E_3^{(4)} = (C^3-C\xi_2+15\xi_3)(a/L)^3E^{(1)} \quad (5.14)$$

in the limit $\epsilon\to 0+$, and

$$E_4^{(4)} = -E^{(1)}\tfrac{1}{3}(8\pi a\Omega^{-1})^3\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' (k_1^2+k_2^2+k_3^2)^{-1}$$
$$\times[k_1^{-2}\cos(k_1\epsilon)\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon)+\text{symm.}]$$
$$\times[k_1^{-2}\cos(\tfrac{1}{2}k_1\epsilon)+\text{symm.}]. \quad (5.15)$$

In (5.15), each component of each $\mathbf{k}$ is of the form $2\pi L^{-1}\times$(integer), and the prime means the omission of those $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$ that makes any one of the energy denominators vanish.

There remains the rather complicated task of finding the behavior of $E_4^{(4)}$ when $\epsilon \ll L$. Only the leading term will be calculated here. Consider first the sum

$$\Sigma_1' = \sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (k_1^2+k_2^2+k_3^2)^{-1}k_1^{-4} \times \cos k_1\epsilon \cos\tfrac{1}{2}k_1\epsilon \cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon). \quad (5.16)$$

Let

$$\mathbf{k}_4 = \mathbf{k}_2 - \mathbf{k}_3, \quad (5.17)$$

then

$$\Sigma_1' = 2 \sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (3k_1^2+k_4^2)^{-1}k_1^{-4} \times \cos k_1\epsilon \cos\tfrac{1}{2}k_1\epsilon \cos\tfrac{1}{2}k_4\epsilon. \quad (5.18)$$

Since the terms with $\mathbf{k}_4=\mathbf{0}$ do not contribute to the leading term, they may be omitted. Furthermore, when the decomposition

$$(3k_1^2+k_4^2)^{-1} = k_4^{-2} - 3k_1^2k_4^{-2}(3k_1^2+k_4^2)^{-1} \quad (5.19)$$

is used in (5.18), those terms coming from k_4^{-2} again do not contribute to the leading term. Therefore

$$\Sigma_1' \sim -6 \sum_{\substack{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0 \\ \mathbf{k}_4\neq 0}}' (3k_1^2+k_4^2)^{-1}k_1^{-2}k_4^{-2} \times \cos k_1\epsilon \cos\tfrac{1}{2}k_1\epsilon \cos\tfrac{1}{2}k_4\epsilon. \quad (5.20)$$

This may next be replaced by the integral

$$\Sigma_1' \sim -\tfrac{3}{4}\Omega^2(2\pi)^{-6}\int d^3\mathbf{k}_1 d^3\mathbf{k}_4 (3k_1^2+k_4^2)^{-1}k_1^{-2}k_4^{-2} \times \cos k_1\epsilon \cos\tfrac{1}{2}k_1\epsilon \cos\tfrac{1}{2}k_4\epsilon, \quad (5.21)$$

where the domain of integration is $k_1 > L^{-1}$, $k_4 > L^{-1}$. Now it is straightforward to get the result that as $\epsilon/L \to 0$

$$\Sigma_1' = -\Omega^2(2\pi)^{-6}[2\pi^3\sqrt{3}\ln(L/\epsilon)+O(1)]. \quad (5.22)$$

The other part of the sum

$$\Sigma_2' = \sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (k_1^2+k_2^2+k_3^2)^{-1}k_1^{-2}k_2^{-2} \times \cos k_1\epsilon \cos\tfrac{1}{2}k_2\epsilon \cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon) \quad (5.23)$$

may be replaced immediately by the integral

$$\Sigma_2' \sim \tfrac{1}{2}\Omega^2(2\pi)^{-6}\int d^3\mathbf{k}_1 d^3\mathbf{k}_2 \times (k_1^2+k_2^2-\mathbf{k}_1\cdot\mathbf{k}_2)^{-1}k_1^{-2}k_2^{-2}, \quad (5.24)$$

where the domain of integration is $L^{-1}<k_1<\epsilon^{-1}$, $L^{-1}<k_2<\epsilon^{-1}$. The angular integral may be evaluated to give

$$\Sigma_2' \sim \Omega^2(2\pi)^{-4}\int_{L^{-1}}^{\epsilon^{-1}} dk_1dk_2(k_1k_2)^{-1} \times \ln\frac{k_1^2+k_2^2+k_1k_2}{k_1^2+k_2^2-k_1k_2}. \quad (5.25)$$

Introduction of the variable $x=k_2/k_1$ yields the result

$$\Sigma_2' \sim 2\Omega^2(2\pi)^{-4}\int_{\epsilon/L}^{1} \frac{dx}{x} \ln\frac{Lx}{\epsilon} \ln\frac{1+x+x^2}{1-x+x^2}. \quad (5.26)$$

Since the integral

$$\int_0^1 \frac{dx}{x} \ln x \ln\frac{1+x+x^2}{1-x+x^2}$$

is convergent, a contour integration gives finally for $\epsilon/L \to 0$

$$\Sigma_2' = \Omega^2(2\pi)^{-4}[\ln(L/\epsilon)\pi^2/3+O(1)]. \quad (5.27)$$

The substitution of (5.16), (5.22), (5.23), and (5.27) in (5.15) yields

$$E_4^{(4)} = -E^{(1)}(a/L)^3 \times[8(8\pi/3-2\sqrt{3})\ln(L/\epsilon)+O(1)]. \quad (5.28)$$

In this calculation ϵ^{-1} acts as a high-momentum cutoff. Since, in the actual problem of hard spheres, the only quantity of high momentum is a^{-1}, the form of the correct expression for the three-body ground-state energy may be expected to be

$$24\pi a\Omega^{-1}\{1+C(a/L)+(C^2+\xi_2)(a/L)^2 +(a/L)^3[(C^3-C\xi_2+15\xi_3 -8(8\pi/3-2\sqrt{3})\ln(L/a)+\mathcal{E}_3]+o[(a/L)^3]\}, \quad (5.29)$$

where (5.6) and (5.14) have been used. In (5.29), $\mathcal{E}_3$ is a number that cannot be determined by the method of the pseudopotential. A comparison of (5.28) and (5.29) gives the following interpretation of the sum in (5.15)

$$\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (k_1^2+k_2^2+k_3^2)^{-1} \times[k_1^{-2}\cos(k_1\epsilon)\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon)+\text{symm.}] \times[k_1^{-2}\cos\tfrac{1}{2}k_1\epsilon+\text{symm.}] \to 3\Omega^2(4\pi)^{-3}[(8\pi/3-2\sqrt{3})\ln(L/a)-\mathcal{E}_3/8]. \quad (5.30)$$

This interpretation is to be used in the N-body problem.

6. GROUND-STATE ENERGY PER PARTICLE—CONTINUED

The asymptotic forms of α_k and E_k are, as $k\to\infty$ and $\xi=1$,

$$\alpha_k \sim 4\pi a\rho k^{-2}, \quad (6.1)$$

and

$$E_k \sim k^2, \quad (6.2)$$

as seen from (3.21), (4.6), (4.7), and (4.19). Furthermore

$$\bar{\alpha}_k = \alpha_k \cos k\epsilon. \quad (6.3)$$

Therefore, when the three momenta are all large, the summand of ΔE_2 as expressed in (4.18) behaves the same as that of the left-hand side of (5.30), except for a numerical factor. To make a more detailed comparison, consider first the difference

$$\Delta_1 = \sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (k_1^2+k_2^2+k_3^2)^{-1}[k_1^{-4}-(4\pi a\rho)^{-2}\alpha_{k_1}^2] \times \cos k_1\epsilon \cos\tfrac{1}{2}k_1\epsilon \cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon). \quad (6.4)$$

This quantity is studied in Appendix A. The result there is

$$\Delta_1 = \tfrac{1}{8}\Omega^2(2\pi)^{-3}[-2\sqrt{3}\ln(12\pi a\rho)^{\frac{1}{2}}L+C_1] \quad (6.5)$$

in the limit $\epsilon \to 0+$ and Ω large. C_1 is a number defined in Appendix A. Next consider the difference

$$\Delta_2 = \sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (k_1^2+k_2^2+k_3^2)^{-1} \times[k_1^{-2}k_2^{-2}-(4\pi a\rho)^{-2}\alpha_{k_1}\alpha_{k_2}]\cos k_1\epsilon \cos\tfrac{1}{2}k_2\epsilon \times\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon). \quad (6.6)$$

In view of (6.1), the limit $\epsilon \to 0+$ may be taken under the summation sign. Thus

$$\Delta_2 = \sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (k_1^2+k_2^2+k_3^2)^{-1} \times[k_1^{-2}k_2^{-2}-(4\pi a\rho)^{-2}\alpha_{k_1}\alpha_{k_2}]. \quad (6.7)$$

As a consequence of (5.27), Δ_2 must be of the form, for large Ω,

$$\Delta_2 = \Omega^2(2\pi)^{-3}[\tfrac{1}{6}\pi\ln(12\pi a\rho)^{\frac{1}{2}}L+C_2], \quad (6.8)$$

where C_2 is a number defined by (6.8). Equations (6.6), (6.8), and (5.30) then give the interpretation

$$(4\pi a\rho)^{-2}\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}' (k_1^2+k_2^2+k_3^2)^{-1} \times[\bar{\alpha}_{k_1}\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon)+\text{symm.}] \times[\alpha_{k_1}\cos\tfrac{1}{2}k_1\epsilon+\text{symm.}]$$
$$\to -3\Omega^2(4\pi)^{-3}[(\tfrac{4}{3}\pi-\sqrt{3})\ln(12\pi a^3\rho)+\tfrac{1}{8}\mathcal{E}_3+C_1+16C_2]. \quad (6.9)$$

Note that $\ln L$ does not appear in (6.9). With (6.9), it is possible to write ΔE_2 in the limit $\Omega \to \infty$ and $\epsilon \to 0+$ explicitly as follows:

$$\Delta E_2 = \Delta E_{21}+\Delta E_{22}+\Delta E_{23}, \quad (6.10)$$

where

$$\Delta E_{21} \to 32\pi a^4\rho^2 N[(\tfrac{4}{3}\pi-\sqrt{3})\ln(12\pi a^3\rho) +\tfrac{1}{8}\mathcal{E}_3+C_1+16C_2], \quad (6.11)$$

$$\Delta E_{22} = -\frac{2a^2N}{3\pi^4}\int\int\int d^3\mathbf{k}d^3\mathbf{k}'d^3\mathbf{k}''\delta(\mathbf{k}+\mathbf{k}'+\mathbf{k}'') \times[\alpha_k+\alpha_{k'}+\alpha_{k''}]^2[(E_k+E_{k'}+E_{k''})^{-1}(1-\alpha_k^2)^{-1} \times(1-\alpha_{k'}^2)^{-1}(1-\alpha_{k''}^2)^{-1}-(k^2+k'^2+k''^2)^{-1}], \quad (6.12)$$

and

$$\Delta E_{23} = \frac{2a^2N}{3\pi^4}\int\int\int d^3\mathbf{k}d^3\mathbf{k}'d^3\mathbf{k}''\delta(\mathbf{k}+\mathbf{k}'+\mathbf{k}'') \times(E_k+E_{k'}+E_{k''})^{-1}(1-\alpha_k^2)^{-1}(1-\alpha_{k'}^2)^{-1} \times(1-\alpha_{k''}^2)^{-1}(\alpha_{k'}\alpha_{k''}+\alpha_{k''}\alpha_{k'}+\alpha_k\alpha_{k'}) \times(2\alpha_k+2\alpha_{k'}+2\alpha_{k''}-\alpha_{k'}\alpha_{k''}-\alpha_{k''}\alpha_k-\alpha_k\alpha_{k'}). \quad (6.13)$$

In (6.12) and (6.13), ϵ may be put to zero in α_k. There only remains a slight simplification of these formulas:

$$\Delta E_{22} = -\frac{16a^2N}{3\pi^2}\int_0^\infty dk\int_0^\infty dk'\int^\infty dk''\, kk'k''U(k,k',k'') \times(\alpha_k+\alpha_{k'}+\alpha_{k''})^2[(E_k+E_{k'}+E_{k''})^{-1}(1-\alpha_k^2)^{-1} \times(1-\alpha_{k'}^2)^{-1}(1-\alpha_{k''}^2)^{-1}-(k^2+k'^2+k''^2)^{-1}], \quad (6.14)$$

and

$$\Delta E_{23} = \frac{16a^2N}{3\pi^2}\int_0^\infty dk\int_0^\infty dk'\int^\infty dk''\, kk'k''U(k,k',k'') \times(E_k+E_{k'}+E_{k''})^{-1}(1-\alpha_k^2)^{-1}(1-\alpha_{k'}^2)^{-1} \times(1-\alpha_{k''}^2)^{-1}(\alpha_{k'}\alpha_{k''}+\alpha_{k''}\alpha_k+\alpha_k\alpha_{k'}) \times(2\alpha_k+2\alpha_{k'}+2\alpha_{k''}+\alpha_{k'}\alpha_{k''}-\alpha_{k''}\alpha_k-\alpha_k\alpha_{k'}), \quad (6.15)$$

where $U(k,k',k'')=1$ if the numbers k, k', k'' can form a triangle, and $=0$ otherwise. For dimensional reasons, $\Delta E_{22}+\Delta E_{23}$ is of the form

$$\Delta E_{22}+\Delta E_{23} = 4\pi a^4\rho^2 NC_3, \quad (6.16)$$

where C_3 is a dimensionless number. Finally, let

$$\mathcal{C} = 8C_1+128C_2+C_3+(128/9\pi), \quad (6.17)$$

then it follows from (4.14) and (6.10) that

$$E_0 = \langle 0|H'|0\rangle+\Delta E_2 = 4\pi a\rho N\left[1+\frac{128}{15\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}} +8(\tfrac{4}{3}\pi-\sqrt{3})(a^3\rho)\ln(12\pi a^3\rho)+(a^3\rho)(\mathcal{E}_3+\mathcal{C})\right]. \quad (6.18)$$

Note that the three-body energy $\mathcal{E}_3$ of (3.72) has not been explicitly found. On the other hand, $\mathcal{C}$ is known in principle by (6.17) in terms of C_1, C_2, and C_3, which in turn are defined in Appendix A, Eq. (6.8), and Eqs. (6.14–16), respectively.

7. PROPERTIES OF THE GROUND STATE

In this section, a few simple properties of the ground state are to be studied.

A. The Depletion Factor ξ

First the formula (4.5) may be improved. From (3.40), it follows that

$$\langle 0|a_0^*a_0|0\rangle = N-\sum_{\mathbf{k}\neq 0}\alpha_k\bar{\alpha}_k(1-\alpha_k\bar{\alpha}_k)^{-1} = N\left[1-\frac{8}{3\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}}\xi^{\frac{3}{2}}\right] \quad (7.1)$$

as $\epsilon \to 0+$ and Ω large. Next it is necessary to calculate the further depletion due to the creation of phonons.

The one-phonon states have the property

$$\langle 0|a_0{}^*a_0|0\rangle-\langle 1_{\mathbf{k}}|a_0{}^*a_0|1_{\mathbf{k}}\rangle =\langle 1_{\mathbf{k}}|a_{\mathbf{k}}{}^*a_{\mathbf{k}}|1_{\mathbf{k}}\rangle-\langle 0|a_{\mathbf{k}}{}^*a_{\mathbf{k}}|0\rangle +\langle 1_{\mathbf{k}}|a_{-\mathbf{k}}{}^*a_{-\mathbf{k}}|1_{\mathbf{k}}\rangle-\langle 0|a_{-\mathbf{k}}{}^*a_{-\mathbf{k}}|0\rangle. \quad (7.2)$$

Since the one-phonon state is explicitly known, it is tedious but straightforward to verify that

$$\langle 1_{\mathbf{k}}|a_{\mathbf{k}}{}^*a_{\mathbf{k}}|1_{\mathbf{k}}\rangle=(1-\alpha_k\bar{\alpha}_k)^{-1}(1+\alpha_k\bar{\alpha}_k), \quad (7.3)$$

and

$$\langle 1_{\mathbf{k}}|a_{-\mathbf{k}}{}^*a_{-\mathbf{k}}|1_{\mathbf{k}}\rangle=2\alpha_k\bar{\alpha}_k(1-\alpha_k\bar{\alpha}_k)^{-1}. \quad (7.4)$$

Accordingly

$$\langle 0|a_0{}^*a_0|0\rangle-\langle 1_{\mathbf{k}}|a_0{}^*a_0|1_{\mathbf{k}}\rangle=(1-\alpha_k\bar{\alpha}_k)^{-1}(1+\alpha_k\bar{\alpha}_k). \quad (7.5)$$

A perturbation calculation with (4.18) then yields

$$\begin{aligned} N\xi-\langle 0|a_0{}^*a_0|0\rangle &=-\sum_{\substack{k>k'>k''>0\\ \mathbf{k}+\mathbf{k}'+\mathbf{k}''=0}} 256\pi^2a^2\rho\Omega^{-1}(E_k+E_{k'}+E_{k''})^{-2} \\ &\times(1-\alpha_k\bar{\alpha}_k)^{-1}(1-\alpha_{k'}\alpha_{k'})^{-1}(1-\alpha_{k''}\bar{\alpha}_{k''})^{-1} \\ &\times[(1-\alpha_k\bar{\alpha}_k)^{-1}(1+\alpha_k\bar{\alpha}_k)+\text{symm.}] \\ &\times[\bar{\alpha}_k\bar{\alpha}_{k'}\cos(\tfrac{1}{2}k''\epsilon)-\bar{\alpha}_{k''}\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|\epsilon)+\text{symm.}] \\ &\times[-\alpha_{k''}\cos(\tfrac{1}{2}k''\epsilon)+\alpha_k\alpha_{k'}\cos(\tfrac{1}{2}|\mathbf{k}-\mathbf{k}'|\epsilon)+\text{symm.}]. \end{aligned} \quad (7.6)$$

Because of the extra energy denominator, the limit $\epsilon\to 0+$ may be taken directly here. The result for $\Omega\to\infty$ and $\epsilon\to 0+$ is

$$\begin{aligned} \xi=1-\frac{8}{3\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}}+\frac{32}{3\pi}a^3\rho-\frac{16a^2}{3\pi} &\times\int_0^\infty dk\int_0^\infty dk'\int_0^\infty dk''\, kk'k''U(k,k',k'') \\ &\times(E_k+E_{k'}+E_{k''})^{-2}(1-\alpha_k{}^2)^{-1}(1-\alpha_{k'}{}^2)^{-1} \\ &\times(1-\alpha_{k''}{}^2)^{-1}[(1-\alpha_k{}^2)^{-1}(1+\alpha_k{}^2)+\text{symm.}] \\ &\times(\alpha_k+\alpha_{k'}+\alpha_{k''}-\alpha_{k'}\alpha_{k''}-\alpha_{k''}\alpha_k-\alpha_k\alpha_{k'})^2, \end{aligned} \quad (7.7)$$

where U is defined after (6.15). Note that no logarithm term appears in (7.7). As before, in the α_k under the integral sign, it is understood that $\epsilon=0$ and $\xi=1$.

B. Three-Particle Wave Function

In the work of Lee, Huang, and Yang,[3] the ground-state wave function is expressed in terms of a two-particle function

$$f(r)=-\frac{1}{8\pi^3\rho}\int d^3\mathbf{k}\,\alpha_k e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (7.8)$$

It is noted there that terms of the form

$$f(r_{12})f(r_{13})$$

are missing in the wave function. In the present calculation, due to the admixing of the three-phonon states, a certain three-particle function takes the place of the combination $f(r_{12})f(r_{13})$+symm. It is the purpose here to make a partial study of this three-particle function.

A phonon does not differ very much from a free particle if its momentum is much larger than $(a\rho)^{\frac{1}{2}}$. This approximation may be used if the three relative distances are much less than $(a\rho)^{-\frac{1}{2}}$. In view of the difficulties arising from the three-body problem, the results are not expected to be valid when the relative distances are of the order of a. Thus it is hereby assumed that

$$a\ll r_{23},r_{31},r_{12}\ll(a\rho)^{-\frac{1}{2}}. \quad (7.9)$$

Under this assumption, define the required function by

$$f_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) =-N^{-\frac{3}{2}}\sum_{\mathbf{k}+\mathbf{k}'+\mathbf{k}''=0}{}' \exp[i(\mathbf{k}\cdot\mathbf{r}_1+\mathbf{k}'\cdot\mathbf{r}_2+\mathbf{k}''\cdot\mathbf{r}_3)] \times\langle 1_{\mathbf{k}},1_{\mathbf{k}'},1_{\mathbf{k}''}|H'|0\rangle(E_k+E_{k'}+E_{k''})^{-1}. \quad (7.10)$$

Since only momenta larger than $(a\rho)^{\frac{1}{2}}$ are of concern, (4.16) simplifies greatly with (6.1) and (6.3). With ϵ put to zero, the result is

$$\langle 1_{\mathbf{k}},1_{\mathbf{k}'},1_{\mathbf{k}''}|H'|0\rangle \sim-64\pi^2a^2\rho\Omega^{-1}N^{\frac{1}{2}}(k^{-2}+k'^{-2}+k''^{-2}). \quad (7.11)$$

Therefore, as $\Omega\to\infty$,

$$\begin{aligned} f_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) &=\pi^{-4}a^2\int\int\int d^3\mathbf{k}_1d^3\mathbf{k}_2d^3\mathbf{k}_3\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3) \\ &\times(k_1{}^{-2}+k_2{}^{-2}+k_3{}^{-2})(k_1{}^2+k_2{}^2+k_3{}^2)^{-1} \\ &\times\exp[i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2+\mathbf{k}_3\cdot\mathbf{r}_3)]. \end{aligned} \quad (7.12)$$

This integral is explicitly evaluated in Appendix B. The result is

$$f_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=8\pi^{-1}3^{-\frac{3}{2}}a^2[r_1'^{-1}(\gamma^2-r_1'^2)^{-\frac{1}{2}} \times\sin^{-1}(r_1'/\gamma)+\text{symm.}], \quad (7.13)$$

where

$$\mathbf{r}_i'=\mathbf{r}_i-\tfrac{1}{3}(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3), \quad (7.14)$$

and γ is defined in (B.15). Under the assumption (7.9) the "missing" terms are

$$f(r_{12})f(r_{13})+\text{symm.}=a^2[|\mathbf{r}_1-\mathbf{r}_2|^{-1}|\mathbf{r}_1-\mathbf{r}_2|^{-1}+\text{symm.}]. \quad (7.15)$$

Thus it may be seen that $f_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ is not quantitatively close to $f(r_{12})f(r_{13})$+symm.

The conclusion is then reached that even at low densitites, the ground-state wave function is not of the form

$$\prod_{i<j}B(r_{ij}). \quad (7.16)$$

In particular, it seems unprofitable to push any further the procedure of Aviles,[10] who calculated the ground-state energy per particle by a variational formula using a trial wave function of the form (7.16).

C. Pair Distribution Function

The pair distribution function, normalized to be 1 at infinite distance, is defined by

$$D(r)=\rho^{-2}\langle G|\psi^*(0)\psi^*(\mathbf{r})\psi(0)\psi(\mathbf{r})|G\rangle \tag{7.17}$$

for the ground state, where $|G\rangle$ is the ground-state wave function. For the determination of $D(r)$, the following formulas are of use:

$$\langle 1_{\mathbf{k}}|a_{\mathbf{k}}a_{-\mathbf{k}}|1_{\mathbf{k}}\rangle=-2\alpha_k(1-\alpha_k\bar{\alpha}_k)^{-1}, \tag{7.18}$$

and

$$\langle 1_{\mathbf{k}}|a_{\mathbf{k}}^*a_{-\mathbf{k}}^*|1_{\mathbf{k}}\rangle=-2\bar{\alpha}_k(1-\alpha_k\bar{\alpha}_k)^{-1}. \tag{7.19}$$

As in the calculation of ξ, it is permissible for the present purpose to set $\epsilon=0$ at the beginning; in particular, $\alpha_k=\bar{\alpha}_k$. Following Lee, Huang, and Yang,[3] define

$$F(r)=\frac{1}{8\pi^3\rho}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}\langle G|a_{\mathbf{k}}^*a_{\mathbf{k}}|G\rangle, \tag{7.20}$$

and

$$G(r)=\frac{1}{8\pi^3\rho}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}\langle G|a_{\mathbf{k}}a_{-\mathbf{k}}|G\rangle$$
$$=\frac{1}{8\pi^3\rho}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}\langle G|a_{\mathbf{k}}^*a_{-\mathbf{k}}^*|G\rangle. \tag{7.21}$$

It follows from (7.6) that

$$F(r)=\frac{1}{8\pi^3\rho}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}\times\left[\frac{\alpha_k^2}{1-\alpha_k^2}+\frac{16a^2\rho}{\pi}\frac{1+\alpha_k^2}{1-\alpha_k^2}\phi(k)\right], \tag{7.22}$$

where

$$\phi(k)=\int d^3\mathbf{k}'[(E_k+E_{k'}+E_{k''})^{-2}(1-\alpha_k^2)^{-1}\times(1-\alpha_{k'}^2)^{-1}(1-\alpha_{k''}^2)^{-1}(\alpha_k+\alpha_{k'}+\alpha_{k''}-\alpha_{k'}\alpha_{k''}-\alpha_{k''}\alpha_k-\alpha_k\alpha_{k'})^2]_{\mathbf{k}''=\mathbf{k}+\mathbf{k}'}. \tag{7.23}$$

Similarly, it follows from (7.18) or (7.19) that

$$G(r)=\frac{1}{8\pi^3\rho}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}\times\left[\frac{-\alpha_k^2}{1-\alpha_k^2}+\frac{16a^2\rho}{\pi}\frac{-2\alpha_k}{1-\alpha_k^2}\phi(k)\right]. \tag{7.24}$$

In addition to $F(r)$ and $G(r)$, the following function is also needed:

$$H(r)=\frac{N^{\frac{1}{2}}}{(8\pi^3\rho)^2}\int\int d^3\mathbf{k}d^3\mathbf{k}'\, e^{i\mathbf{k}\cdot\mathbf{r}}\langle G|a_{\mathbf{k}+\mathbf{k}'}^*a_{\mathbf{k}}a_{\mathbf{k}'}|G\rangle$$
$$=\frac{N^{\frac{1}{2}}}{(8\pi^3\rho)^2}\int\int d^3\mathbf{k}d^3\mathbf{k}'\, e^{i\mathbf{k}\cdot\mathbf{r}}\times\langle G|a_{\mathbf{k}}^*a_{\mathbf{k}'}^*a_{\mathbf{k}+\mathbf{k}'}|G\rangle. \tag{7.25}$$

A calculation quite similar to the above gives

$$H(r)=-\frac{a}{4\pi^5\rho}\int\int\int d^3\mathbf{k}d^3\mathbf{k}'d^3\mathbf{k}''\,\delta(\mathbf{k}+\mathbf{k}'+\mathbf{k}'')e^{i\mathbf{k}\cdot\mathbf{r}}\times(E_k+E_{k'}+E_{k''})^{-1}(1-\alpha_k^2)^{-1}(1-\alpha_{k'}^2)^{-1}\times(1-\alpha_{k''}^2)^{-1}(\alpha_{k''}-\alpha_k\alpha_{k'})(\alpha_k+\alpha_{k'}+\alpha_{k''}-\alpha_{k'}\alpha_{k''}-\alpha_{k''}\alpha_k-\alpha_k\alpha_{k'}). \tag{7.26}$$

In terms of the functions $F(r)$, $G(r)$ and $H(r)$, the pair distribution function of (7.17) may be written as

$$D(r)=1+2\xi[F(r)+G(r)]+[F(r)]^2+[G(r)]^2+4H(r). \tag{7.27}$$

However, note that except for the exponential factor, $H(r)$ is very similar to the ΔE_2 of (4.18). Therefore, due to the complication arising from the three-body problem, (7.26) for $H(r)$ is inaccurate for $r\sim a$. Compared with the result of Lee, Huang, and Yang, the more complicated formula (7.27) gives no extra information for $r\sim a$, but is probably more accurate for $a\ll r$.

It remains to evaluate $D(r)$ approximately for $(a\rho)^{-\frac{1}{2}}\ll r$. Since

$$F(r)+G(r)=\frac{1}{8\pi^3\rho}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}\times\left[\frac{-\alpha_k}{1+\alpha_k}+\frac{16a^2\rho}{\pi}\frac{1}{(1+\alpha_k)^2}\bar{\phi}(k)\right], \tag{7.28}$$

where $\bar{\phi}(k)$ is that of (C.1), it follows from (3.13) that as $r\rightarrow\infty$

$$F(r)+G(r)\rightarrow -8\frac{r_0^4}{r^4}\left(\frac{a^3\rho}{\pi}\right)^{\frac{1}{2}}\left[1-\frac{8}{3}\left(\frac{a^3\rho}{\pi}\right)^{\frac{1}{2}}\right], \tag{7.29}$$

where

$$r_0=(8\pi a\rho)^{-\frac{1}{2}}. \tag{7.30}$$

On the other hand, in terms of the $\bar{\phi}'(k)$ of (C.14), $H(r)$ of (7.26) is

$$H(r)=-\frac{a}{4\pi^5\rho}\int d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}(1-\alpha_k^2)^{-1}\bar{\phi}'(k). \tag{7.31}$$

Application of (C.18) gives, as $r\rightarrow\infty$,

$$H(r)\rightarrow -\left(\frac{a^3\rho}{\pi}\right)\frac{128r_0^4}{r^4}\left(\frac{4}{3}-\frac{\pi}{2}\right). \tag{7.32}$$

[10] J. B. Aviles, Jr., doctorate dissertation, Johns Hopkins University, 1958 (unpublished).

So far as the terms $[F(r)]^2$ and $[G(r)]^2$ in (7.27) are concerned, it is sufficient to use the result of Lee, Huang, and Yang[3] that as $r\to\infty$

$$F(r)\to(\pi^2\rho r_0 r^2)^{-1},\qquad G(r)\to-(\pi^2\rho r_0 r^2)^{-1}; \tag{7.33}$$

therefore

$$[F(r)]^2+[G(r)]^2\to 1024\frac{r_0^4}{r^4}\left(\frac{a^3\rho}{\pi}\right). \tag{7.34}$$

Finally the substitution of (7.29), (7.32), and (7.34) into (7.27) gives, as $r\to\infty$,

$$D(r)\neq 1-\frac{r_0^4}{r^4}\left[16\left(\frac{a^3\rho}{\pi}\right)^{\frac{1}{2}}\right]\times\left[1-\left(16\pi+\frac{80}{3}\right)\left(\frac{a^3\rho}{\pi}\right)^{\frac{1}{2}}\right]. \tag{7.35}$$

This is the desired answer.

D. Sound Speed

Although strictly not a property of the ground state, the speed of propagation of a compressional wave in the limit of infinite wavelength is related to the ground-state energy per particle.[3] Thus it follows from (6.18) that this speed is

$$(16\pi a\rho)^{\frac{1}{2}}\left\{1+\frac{8}{\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}}+12(\tfrac{4}{3}\pi-\sqrt{3})a^3\rho\ln(12\pi a^3\rho)+(a^3\rho)[\tfrac{3}{2}(\mathcal{E}_3+\mathcal{C})+10(\tfrac{4}{3}\pi-\sqrt{3})-32/\pi]\right\}. \tag{7.36}$$

8. DISCUSSIONS

Since the preceding calculation is concerned with an improvement over the results of Lee, Huang, and Yang,[3] it only remains to discuss a few miscellaneous topics peculiar to these higher order terms.

A. Although this calculation has been carried out only for the case of hard-sphere interaction, it also applies to any repulsive interaction of short range. In fact, the only modifications are: (a) $\mathcal{E}_3$ is in general different, and (b) the length a appearing in the calculation is to be interpreted as scattering length of the two-body potential. In particular, the logarithm term of (6.18) appears in the more general case.

B. This logarithm term may be obtained by an argument as follows. From (5.29) for the three-body problem, the three-body ground-state energy has a term

$$-192\pi[(8/3)\pi-2\sqrt{3}]a^4L^{-6}\ln(L/a).$$

In the logarithm, L^{-1} plays the role of a low-momentum cutoff. Since

$$\binom{N}{3}=N^3/6,$$

for large N, there should be a term of the following form in E_0:

$$-\frac{N^3}{6}192\pi\left(\frac{8}{3}\pi-2\sqrt{3}\right)a^4L^{-6}\ln(L'/a),$$

where L'^{-1} is some low-momentum cutoff. Since this should be proportional to N, L' must be independent of the size of the box. This leaves just one possible choice, namely

$$L'=(a\rho)^{-\frac{1}{2}}.$$

With this choice of L', this energy becomes

$$16\pi[(8/3)\pi-2\sqrt{3}]a^4\rho^2N\ln(a^3\rho),$$

which is identical to the logarithm term of (6.18). In fact, this is the argument originally used to get this term, before the present calculation was carried out. However, it is much more satisfying to see the explicit cancellation of L under the logarithm sign, as exhibited in (6.9).

C. It may also be noted that no logarithm appears in the depletion factor ξ of (7.7). Thus the logarithm term of the ground-state energy does not come from the depletion of the single-particle $k=0$ state.

D. Contrary to $\mathcal{C}$, no formula has been found for the number $\mathcal{E}_3$. After repeated failure to find $\mathcal{E}_3$, the author conjectures that $\mathcal{E}_3$ cannot be expressed in terms of a finite number of integrals involving only well-known functions.

E. If an unknown number $\mathcal{E}_3$ has to be introduced for the ground-state energy per particle, why is ξ of (7.7) well defined? The reason is as follows. The complication due to the three-body problem implies that the matrix elements of (4.16) and (4.17) are inaccurate for any k of the order of a^{-1}. For large k, the energy behaves like k^2 but the depletion behaves like 1, from (7.5). Thus the unknown region of large momenta contributes much more to the ground-state energy per particle than to the depletion factor ξ. To the order calculated, it turns out that the contribution is of importance for the former quantity but not for the latter.

F. The existence of a sound speed (7.36) implies the absence of an energy gap immediately above the ground state. How can this be verified directly? Even though the phonon spectrum is unstable due to the three-phonon perturbation, for a given Ω the one-phonon state with a momentum of $2\pi/L$ is stable. It is possible to modify the present calculation to find the energy of this state. Here it is important to note that the ground-state depletion factor for this state is different from ξ. When this is taken into account, a very tedious calculation yields the result that there is no energy gap to order $a\rho(a^3\rho)^{\frac{1}{2}}$.

G. So far as the asymptotic behavior of the pair distribution function $D(r)$ is concerned, although the first two terms of the coefficient of $(r_0/r)^4$ are given in (7.35), there seem to exist no proof that it is indeed of the form $1+O[(r_0/r)^4]$ as $r\to\infty$. In particular, a term of the form $(\rho a^3)^{\frac{3}{2}}(r_0/r)^4\ln(r/r_0)$ has not been excluded.

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APPENDIX A

In this Appendix, the quantity Δ_1 defined by (6.4) is studied. Since $\epsilon\to 0+$ eventually, two of the cosine factors are ineffective; thus

$$\Delta_1=\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' (k_1^2+k_2^2+k_3^2)^{-1}\times[k_1^{-4}-(4\pi a\rho)^{-2}\alpha_{k_1}{}^2]\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon). \quad (A.1)$$

The first part of Δ_1 is identical with the Σ_1' of (5.16). According to (5.18) and (5.19), Δ_1 may be broken up into

$$\Delta_1=\Sigma_{10}'+\Sigma_{11}'+\Sigma_{12}'-\Sigma_1'', \quad (A.2)$$

where

$$\Sigma_{10}'=\sum_{\substack{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0\\ \mathbf{k}_2=\mathbf{k}_3}}{}' (k_1^2+k_2^2+k_3^2)^{-1}k_1^{-4}\times\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon), \quad (A.3)$$

$$\Sigma_{11}'=2\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' k_4^{-2}k_1^{-4}\cos\tfrac{1}{2}k_4\epsilon, \quad (A.4)$$

$$\Sigma_{12}'=-6\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' (3k_1^2+k_4^2)^{-1}k_1^{-2}k_4^{-2}\cos\tfrac{1}{2}k_4\epsilon, \quad (A.5)$$

and

$$\Sigma_1''=(4\pi a\rho)^{-2}\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' (k_1^2+k_2^2+k_3^2)^{-1}\alpha_{k_1}{}^2\times\cos(\tfrac{1}{2}|\mathbf{k}_2-\mathbf{k}_3|\epsilon). \quad (A.6)$$

Here $\mathbf{k}_4$ is that of (5.17). Clearly with (5.7)

$$\Sigma_{10}'=\frac{1}{12}\frac{\Omega^2}{(2\pi)^3}\xi_3. \quad (A.7)$$

For the evaluation of Σ_{11}', define the following variations of the constants C and ξ_2:

$$\xi_2'=\pi^{-2}\sum_{l,m,n=-\infty}^{\infty}[l^2+m^2+(n+\tfrac{1}{2})^2]^{-2}, \quad (A.8)$$

$$\xi_2''=\pi^{-2}\sum_{l,m,n=-\infty}^{\infty}[l^2+(m+\tfrac{1}{2})^2+(n+\tfrac{1}{2})^2]^{-2}, \quad (A.9)$$

$$\xi_2'''=\pi^{-2}\sum_{l,m,n=-\infty}^{\infty}[(l+\tfrac{1}{2})^2+(m+\tfrac{1}{2})^2+(n+\tfrac{1}{2})^2]^{-2}, \quad (A.10)$$

$$C'=\pi^{-1}\lim_{\epsilon\to0+}\sum_{l\ m,n=-\infty}^{\infty}[l^2+m^2+(n+\tfrac{1}{2})^2]^{-1}\times\cos[\epsilon(l^2+m^2+n^2)^{\frac{1}{2}}], \quad (A.11)$$

$$C''=\pi^{-1}\lim_{\epsilon\to0+}\sum_{l,m,n=-\infty}^{\infty}[l^2+(m+\tfrac{1}{2})^2+(n+\tfrac{1}{2})^2]^{-1}\times\cos[\epsilon(l^2+m^2+n^2)^{\frac{1}{2}}], \quad (A.12)$$

and

$$C'''=\pi^{-1}\lim_{\epsilon\to0+}\sum_{l,m,n=-\infty}^{\infty}[(l+\tfrac{1}{2})^2+(m+\tfrac{1}{2})^2+(n+\tfrac{1}{2})^2]^{-1}\times\cos[\epsilon(l^2+m^2+n^2)^{\frac{1}{2}}]. \quad (A.13)$$

These constants are related by

$$\xi_2'+\xi_2''+\tfrac{1}{3}\xi_2'''=5\xi_2, \quad (A.14)$$

and

$$C'+C''+\tfrac{1}{3}C'''=C. \quad (A.15)$$

In terms of these constants, Σ_{11}' is, in the limit $\epsilon\to0+$,

$$\Sigma_{11}'=\frac{1}{256}\frac{\Omega^2}{(2\pi)^3}(C\xi_2+3C'\xi_2'+3C''\xi_2''+C'''\xi_2'''). \quad (A.16)$$

In a similar manner, Σ_1'' may be separated into

$$\Sigma_1''=\Sigma_{11}''+\Sigma_{12}'', \quad (A.17)$$

where

$$\Sigma_{11}''=2(4\pi a\rho)^2\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' k_4^{-2}\alpha_{k_1}{}^2\cos\tfrac{1}{2}k_4\epsilon, \quad (A.18)$$

and

$$\Sigma_{12}''=-6(4\pi a\rho)^{-2}\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' (3k_1^2+k_4^2)^{-1}\times k_1^2k_4^{-2}\alpha_{k_1}{}^2\cos\tfrac{1}{2}k_4\epsilon. \quad (A.19)$$

In the limit $\Omega\to\infty$,

$$\frac{1}{\Omega}\sum_k\alpha_k{}^2\to\frac{1}{2\pi^2}\int_0^\infty\alpha_k{}^2k^2dk=\frac{32}{105\pi^2}(4\pi a\rho)^{\frac{3}{2}}. \quad (A.20)$$

Therefore Σ_{11}' is of the order $\Omega^{5/3}$ as $\Omega\to\infty$ and hence may be omitted. Finally, as $\epsilon\to0$,

$$\Sigma_{12}'-\Sigma_{12}''=-6\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' (3k_1^2+k_4^2)^{-1}k_1^{-2}k_4^{-2}\times[1-(4\pi a\rho)^{-2}k_1^4\alpha_{k_1}{}^2]. \quad (A.21)$$

In order to consider the two terms separately, it is convenient to introduce a high-momentum cutoff for $\mathbf{k}_4$. As $\Omega\to\infty$,

$$\begin{aligned}\Omega^{-2}6\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0}{}' &(3k_1^2+k_4^2)^{-1}k_1^2k_4^{-2}(4\pi a\rho)^{-2}\alpha_{k_1}{}^2\\ &\to\frac{6}{(2\pi)^6}\int d^3\mathbf{k}_2d^3\mathbf{k}_3(3k_1^2+k_4^2)^{-1}k_1^2k_4^{-2}(4\pi a\rho)^{-2}\alpha_{k_1}{}^2\\ &=\frac{3}{16\pi^4}\int_0^K dk_4\int_0^\infty dk_1\, k_1^4(3k_1^2+k_4^2)^{-1}(4\pi a\rho)^{-2}\alpha_{k_1}{}^2\\ &=\frac{\sqrt{3}}{32\pi^3}\left[\ln(12\pi a\rho)^{-\frac{1}{2}}K-\frac{19}{12}+o(1)\right] \quad (A.22)\end{aligned}$$

as $K\to\infty$. On the other hand, in view of (5.22), it is possible to define

$$C_1'=\lim_{N\to\infty}\{\Sigma'[3(l^2+m^2+n^2)+(l'^2+m'^2+n'^2)]^{-1}\times[l^2+m^2+n^2]^{-1}[l'^2+m'^2+n'^2]^{-1}-\pi^3 3^{-\frac{1}{2}}\ln(2\pi N)\},\quad (A.23)$$

where the Σ' extends over l, m, n, l', m', and n' such that $l'^2+m'^2+n'^2<N^2$, and $l+l'$, $m+m'$, $n+n'$ are all even. With (A.22) and (A.23), (A.21) reduces to

$$\Sigma_{12}'-\Sigma_{12}''=-\Omega^2(2\pi)^{-6}[2\sqrt{3}\pi^3\ln(12\pi a\rho)^{\frac{1}{2}}L+6C_1'+(19\sqrt{3}/6)\pi^3].\quad (A.24)$$

Now (A.7), (A.16), and (A.24) may be substituted into (A.2) to yield

$$\Delta_1=\frac{1}{8}\frac{\Omega^2}{(2\pi)^3}[-2\sqrt{3}\ln(12\pi a\rho)^{\frac{1}{2}}L+C_1],\quad (A.25)$$

where

$$C_1=\tfrac{2}{3}\xi_3+\frac{1}{32}(C\xi_2+3C'\xi_2'+3C''\xi_2''+C'''\xi_2''')-6\pi^{-3}C_1'-\frac{19\sqrt{3}}{6}.\quad (A.26)$$

APPENDIX B

In this appendix, the following integral, which appears in (7.12), is evaluated:

$$I=\int\int\int d^3\mathbf{k}_1d^3\mathbf{k}_2d^3\mathbf{k}_3\,\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)(k_1^2+k_2^2+k_3^2)^{-1}\times k_1^{-2}\exp[i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2+\mathbf{k}_3\cdot\mathbf{r}_3)].\quad (B.1)$$

When the integral representations

$$\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)=(2\pi)^{-3}\int d^3\mathbf{R}\exp[i\mathbf{R}\cdot(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)]\quad (B.2)$$

and

$$(k_1^2+k_2^2+k_3^2)^{-1}=\int_0^\infty d\zeta\exp[-\zeta(k_1^2+k_2^2+k_3^2)]\quad (B.3)$$

are used in (B.1), I becomes

$$I=(2\pi)^{-3}\int d^3\mathbf{R}\times\int^\infty d\zeta J(\mathbf{R}+\mathbf{r}_1,\zeta)K(\mathbf{R}+\mathbf{r}_2,\zeta)K(\mathbf{R}+\mathbf{r}_3,\zeta),\quad (B.4)$$

where

$$J(\mathbf{R},\zeta)=\int d^3\mathbf{k}\,k^{-2}\exp(i\mathbf{k}\cdot\mathbf{R}-\zeta k^2),\quad (B.5)$$

and

$$K(\mathbf{R},\zeta)=-\frac{\partial}{\partial\zeta}J(\mathbf{R},\zeta).\quad (B.6)$$

The function K may be integrated to give

$$K(\mathbf{R},\zeta)=(\pi/\zeta)^{\frac{3}{2}}\exp(-\tfrac{1}{4}R^2/\zeta),\quad (B.7)$$

and hence

$$J(\mathbf{R},\zeta)=\int_\zeta^\infty(\pi/\zeta')^{\frac{3}{2}}\exp(-\tfrac{1}{4}R^2/\zeta')d\zeta'.\quad (B.8)$$

When (B.7) amd (B.8) are substituted into (B.4), the ζ integral and the angular part of the $\mathbf{R}$ integral may be carried out to give

$$I=2\pi^3 3^{-\frac{3}{2}}r_1^{-1}\int_{-\infty}^\infty dR(R^2+\alpha^2)^{-\frac{1}{2}}(-R+r_1)\times(R^2+Rr_1+\beta^2)^{-1},\quad (B.9)$$

where

$$\alpha^2=\tfrac{1}{3}(r_1^2+r_2^2+r_3^2),\quad (B.10)$$

and

$$\beta^2=\tfrac{1}{2}(r_2^2+r_3^2).\quad (B.11)$$

In (B.9), it has been assumed that $\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3=0$ without loss of generality. The evaluation of the remaining integral is straightforward but tedious. The relation

$$3\alpha^2-2\beta^2-r_1^2=0\quad (B.12)$$

simplifies the calculation greatly. The result is

$$I=8\pi^3 3^{-\frac{3}{2}}r_1^{-1}(2\alpha^2-r_1^2)^{-\frac{1}{2}}\sin^{-1}(2^{-\frac{1}{2}}r_1/\alpha).\quad (B.13)$$

In order to remove the restriction $\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3=0$, it is sufficient to make the following substitution in (B.13):

$$\mathbf{r}_i\to\mathbf{r}_i+\tfrac{1}{3}(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3).\quad (B.14)$$

Under this substitution

$$2\alpha^2\to\gamma^2=\tfrac{2}{3}(r_1^2+r_2^2+r_3^2)+(7/27)(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)^2.\quad (B.15)$$

APPENDIX C

Consider the integral

$$\bar{\phi}(k)=(1-\alpha_k^2)\phi(k)=\int d^3\mathbf{k}'\,M(\mathbf{k},\mathbf{k}'),\quad (C.1)$$

where

$$M(\mathbf{k},\mathbf{k}')=[(E_k+E_{k'}+E_{k''})^{-2}(1-\alpha_{k'}^2)^{-1}\times(1-\alpha_{k''}^2)^{-1}(\alpha_k+\alpha_{k'}+\alpha_{k''}-\alpha_{k'}\alpha_{k''}-\alpha_{k''}\alpha_k-\alpha_k\alpha_{k'})^2]_{\mathbf{k}''=\mathbf{k}+\mathbf{k}'}.\quad (C.2)$$

Assume

$$k\ll(a\rho)^{\frac{1}{2}}.\quad (C.3)$$

When $k'\ll(a\rho)^{\frac{1}{2}}$, the behavior of $M(\mathbf{k},\mathbf{k}')$ is

$$M(\mathbf{k},\mathbf{k}')=(16\pi a\rho\xi)^{-1}(4k'|\mathbf{k}+\mathbf{k}'|)^{-1}.\quad (C.4)$$

When $k\ll k'$, it is convenient to use

$$\mathbf{p}=\mathbf{k}'+\tfrac{1}{2}\mathbf{k},\quad (C.5)$$

and

$$M(\mathbf{k},\mathbf{k}')=[2p(16\pi a\rho\xi+p^2)^{\frac{1}{2}}+k(16\pi a\rho\xi)^{\frac{1}{2}}]^{-2}\times(1-\alpha_p{}^2)^{-2}[1-\alpha_p{}^2-k(4\pi a\rho\xi)^{-\frac{1}{2}}(1-2\alpha_p)]^2$$
$$=[4p^2(p^2+16\pi a\rho\xi)]^{-1}\left[1-\frac{k(16\pi a\rho\xi)^{\frac{1}{2}}}{p(p^2+16\pi a\rho\xi)^{\frac{1}{2}}}-2\frac{k(1-2\alpha_p)}{(4\pi a\rho\xi)^{\frac{1}{2}}(1-\alpha_p{}^2)}\right]. \quad \text{(C.6)}$$

Take a momentum K such that

$$k\ll K\ll(a\rho)^{\frac{1}{2}}, \quad \text{(C.7)}$$

and write (C.1) in the form

$$\bar{\phi}(k)=\bar{\phi}_1(k)+\bar{\phi}_2(k), \quad \text{(C.8)}$$

where

$$\bar{\phi}_1(k)=\int_{p<K}d^3\mathbf{k}'\,M(\mathbf{k}\,\mathbf{k}'), \quad \text{(C.9)}$$

and

$$\bar{\phi}_2(k)=\int_{p>K}d^3\mathbf{k}'\,M(\mathbf{k},\mathbf{k}'). \quad \text{(C.10)}$$

It is then found from (C.4) that

$$\bar{\phi}_1(k)=\frac{\pi}{16\pi a\rho\xi}[K+O(k^2/K)]. \quad \text{(C.11)}$$

On the other hand, $\bar{\phi}_2(k)$ is

$$\bar{\phi}_2(k)=\pi(16\pi a\rho\xi)^{-\frac{1}{2}}\int_{\sinh^{-1}K(16\pi a\rho\xi)^{-\frac{1}{2}}}^{\infty}d\theta\,\mathrm{sech}\theta\times[1-4k(16\pi a\rho\xi)^{-\frac{1}{2}}(1+e^{-2\theta})^{-1}]$$
$$=-\pi K(16\pi a\rho\xi)^{-1}+\tfrac{1}{2}\pi^2(16\pi a\rho\xi)^{-\frac{1}{2}}-4\pi k(16\pi a\rho\xi)^{-1}(\tfrac{1}{4}\pi+\tfrac{1}{2}). \quad \text{(C.12)}$$

Therefore, for $k\ll(a\rho)^{\frac{1}{2}}$, the first two terms of $\bar{\phi}(k)$ are

$$\bar{\phi}(k)=\tfrac{1}{2}\pi^2(16\pi a\rho\xi)^{-\frac{1}{2}}-4\pi k(16\pi a\rho\xi)^{-1}(\tfrac{1}{4}\pi+\tfrac{1}{2}). \quad \text{(C.13)}$$

In (7.26), a function similar to $\bar{\phi}(k)$ appears:

$$\bar{\phi}'(k)=\int d^3\mathbf{k}'\,M'(\mathbf{k},\mathbf{k}') \quad \text{(C.14)}$$

where

$$M'(\mathbf{k},\mathbf{k}')=[(E_k+E_{k'}+E_{k''})^{-1}(1-\alpha_{k'}{}^2)^{-1}\times(1-\alpha_{k''}{}^2)^{-1}(\alpha_{k''}-\alpha_k\alpha_{k'})(\alpha_k+\alpha_{k'}+\alpha_{k''}-\alpha_{k'}\alpha_{k''}-\alpha_{k''}\alpha_k-\alpha_k\alpha_{k'})]_{\mathbf{k}''=\mathbf{k}+\mathbf{k}'}. \quad \text{(C.15)}$$

Again assume (C.3). For $k'\ll(a\rho)^{\frac{1}{2}}$,

$$M'(\mathbf{k},\mathbf{k}')=(16\pi a\rho\xi)^{-1}(2k'|\mathbf{k}+\mathbf{k}'|)^{-1}\times(-|\mathbf{k}+\mathbf{k}'|+k+k'); \quad \text{(C.16)}$$

and for $k\ll k'$

$$M'(\mathbf{k},\mathbf{k}')=[4p^2(p^2+16\pi a\rho\xi)]^{-\frac{1}{2}}\times\left[1-\tfrac{1}{2}\frac{k(16\pi a\rho\xi)^{\frac{1}{2}}}{p(p^2+16\pi a\rho\xi)^{\frac{1}{2}}}-\frac{k(1-2\alpha_p)}{(4\pi a\rho\xi)^{\frac{1}{2}}(1-\alpha_p{}^2)}\right]\times\left[(|\mathbf{k}+\mathbf{k}'|-k')\frac{d}{dp}\alpha_p+(1-\alpha_k)\times\left(\alpha_p+(k'-p)\frac{d}{dp}\alpha_p\right)\right]. \quad \text{(C.17)}$$

The situation here is very similar to the case of $\bar{\phi}(k)$. Thus it is permissible to use (C.17) in (C.14). The result is then

$$\bar{\phi}'(k)=2\pi(1-\alpha_k)[\tfrac{1}{3}(16\pi a\rho\xi)^{\frac{1}{2}}-k(\tfrac{1}{2}\pi-1)]. \quad \text{(C.18)}$$