where $K_\nu(t)=(\pi i/2)e^{i\pi\nu/2}H_\nu^{(1)}(it)$. The conditions for the validity of this expression are given in reference 12 as $\mathrm{Re}(\alpha+\beta)>0$ and $\mathrm{Re}(\rho\pm\mu\pm\nu+1)>0$. However, the sign of ρ in the second condition is incorrect. The basic requirement is that the integral converge,[28] and the expression, Eq. (4.15), for $H_\nu^{(1)}(t)$ for small t can be used to establish the correct limitation on ρ, μ, and ν. Convergence at infinity is assured by the exponential behavior of the K functions at large distances. For the quasidivergent integrals needed in the text, $\alpha=\beta$, and $\mu=\nu$. In these cases, Eq. (A2) simplifies to

$$\int K_\nu^2(t)t^n dt=\frac{2^{n-2}}{\Gamma(1+n)}\Gamma\left(\tfrac{1}{2}+\nu+\frac{n}{2}\right)\times\Gamma^2\left(\frac{1+n}{2}\right)\Gamma\left(\frac{1+n}{2}-\nu\right). \quad \text{(A3)}$$

[28] E. C. Titchmarsh, Proc. London Math. Soc. **2**, 97 (1927).

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Simplified Approach to the Ground-State Energy of an Imperfect Bose Gas

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The well-known first two terms in the asymptotic density series for the ground-state energy of a Bose gas, $E_0=2\pi N\rho a[1+(128/15\sqrt{\pi})(\rho a^3)^{1/2}]$, where a is the scattering length of the pair potential, is ordinarily obtained by summing an infinite set of graphs in perturbation theory. We show here how this same series may be obtained by elementary methods. Our method offers the advantages of simplicity and directness. Another advantage is that the hard-core case can be handled on the same basis as a finite potential, no pseudopotential being required. In fact, the analysis of the hard-core potential turns out to be simpler than for a finite potential, as is the case in elementary quantum mechanics. In an Appendix we discuss the high-density situation and show that for a certain class of potentials Bogoliubov's theory is correct in this limit. Thus, Bogoliubov's theory, which is never correct at low density unless a pseudopotential is introduced, is really a high-density theory.

INTRODUCTION

IMPORTANT and often brilliant theoretical investigations by many workers in the past few years have given us considerable insight into the nature of the ground state and low-lying excited states of a many-particle Bose gas at low density with repulsive pairwise forces. While the intermediate density problem is still unsolved, we at least know now how to begin a consistent expansion (possibly divergent) in the density. In appropriate units[1] we have the following well-known formulas for the ground-state energy, E_0, and the energies of the elementary excitations of long wavelength, $\epsilon(\mathbf{k})$:

$$E_0=2\pi N\rho a\{1+(128/15\sqrt{\pi})(\rho a^3)^{1/2}+\cdots\}, \quad (1.1)$$

$$\epsilon(\mathbf{k})=2(\pi\rho a)^{1/2}k+\cdots, \quad (1.2)$$

where N is the number of particles, $\rho=N/V$ is the density, and $a>0$ is the scattering length of the two-body potential. The omitted higher terms in Eq. (1.1) depend upon the shape of the potential as well as the scattering length; Eq. (1.2) is justified if $k\ll(\rho a)^{1/2}$.

While Eqs. (1.1) and (1.2) may now be regarded as well established and, therefore, elementary, it was not always so. The first attempt to find E_0 was based on perturbation theory. Aside from the fact that perturbation theory cannot be justified in this case (E_0 is enormously greater than the spacing between the unperturbed ground and first excited states), it is easily seen that all terms in the perturbation series beyond the second are divergent for any potential. By this is meant that although the terms are not actually infinite, they are proportional to a higher power of N than the first.

Nevertheless, it was held for a long time that the first term in the perturbation series, viz.,

$$E_0'=2\pi N\rho a', \quad (1.3a)$$

where

$$a'=\frac{1}{4\pi}\int v(\mathbf{x})d^3x, \quad (1.3b)$$

was exact,[2] $v(\mathbf{x})$ being the two-body potential. Equation

[1] $\hbar=1$, $m=1$.

[2] We must be careful to define the meaning of exact and approximate as used in this paper. We are interested in calculating E_0 as a function of density for a given fixed potential; we are, therefore, concerned with an asymptotic series in the density whose coefficients, and, indeed, whose entire form are functionals of the potential. As such, Eq. (1.1) is exact in that it gives correctly the first two terms in an asymptotic series. Equations (1.3) and (1.6) are only approximations to that series. If, on the other hand, we regard the potential as being proportional to some parameter, λ, and if we were interested in a double expansion in ρ *and* λ, then Eqs. (1.3) and (1.6) would be exact. We are not interested in this latter type of series because for a large potential, such as a hard core, it is relatively useless. Indeed, there is no need for such a double series, because it is the burden of this paper, as well as of a good deal of previous work, that it is just as easy to generate the former type of single series as the latter double series.

(1.3) was justified on the grounds that E_0' is the expectation value of the Hamiltonian in the unperturbed ground state and that

$$\lim_{\rho\to 0}\langle\psi_0|\psi\rangle=1, \tag{1.4}$$

where ψ_0 and ψ are, respectively, the normalized unperturbed and exact ground-state functions. Equation (1.4), while seemingly reasonable, is only an approximation. The truth is that the left-hand side of Eq. (1.4) is asymptotically zero for large N, not unity.[3–5] It is quite true that ψ approaches unity (i.e., ψ_0) when *all* particles are far apart, but when two or more particles are close together ψ differs appreciably from ψ_0 and this difference does not vanish in the limit $\rho\to 0$. But it is precisely the region when two particles are close together that is needed for evaluating the potential energy. It might be remarked in passing that E_0' must be an upper bound for E_0, a fact borne out by the Spruch, Rosenberg inequality[6]:

$$a<\frac{1}{4\pi}\int v(\mathbf{x})d^3x=a' \tag{1.5}$$

for all $v(\mathbf{x})$ that have no bound states.

The incorrectness of Eq. (1.3) notwithstanding, it is a good approximation to E_0 for those potentials that are relatively shallow compared to their width. Of course, E_0' is completely nonsense for a potential with a hard core, and this gave rise to the view that the hard-core potential was particularly difficult, requiring special tricks and methods—a curious conclusion in view of the especial simplicity of the hard-core potential for two particles.

With E_0' as a starting point, the next problem was to do something about the divergent terms in the perturbation series. Various methods were introduced which in one way or another consisted in summing up an infinite subset of the terms in the perturbation series. A typical, and especially neat example of this procedure is Bogoliubov's method[7] which characteristically gives as a solution Eq. (1.1) with the scattering length, a, replaced thoughout by a'.

$$E_0'+E_0''=2\pi N\rho a'\times\{1+(128/15\sqrt{\pi})[\rho(a')^3]^{1/2}+\cdots\}. \tag{1.6}$$

The method is extraordinarily reasonable, but fails in that it relies on Eq. (1.4) which, as we have seen, is incorrect owing to a misinterpretation of the limiting process $\rho\to 0$.

The next step was the realization that a' is itself the first term in the Born series for a, and with this as a clue it was then seen that each term in the partial summation of the perturbation series mentioned above was itself the first term in a heirarchy which, though it could not be explicitly summed, could be recognized as the Born series for a.[8–10]

Thus, by a very complicated twofold summation of infinite sets of graphs, Eq. (1.1) was finally obtained. At this point, mention must be made of the important work of Lee, Huang, and Yang[11] on the hard-sphere Bose gas. For this problem a', of course, does not exist and so one could not arrive at Eq. (1.6) as a first approximation to Eq. (1.1). But by using the pseudopotential (or alternatively the exact formulation in momentum space given by the author[12]) and then Bogoliubov's method, these authors were able to arrive at Eq. (1.1). At first sight it seems very surprising that Bogoliubov's method, which is never correct and indeed gets worse the deeper the potential, should give the correct answer in the case of an infinite repulsive core. The reason is that by using the pseudopotential as a starting point one has partially solved the problem already, and in fact what has been done is to reverse the order of summing the twofold infinite series mentioned above. An important point to note is that only after Lee, Huang, and Yang had successfully come to grips with the infinite repulsive core, and thereby clearly demonstrated that the scattering length and not a' is the relevant parameter, was progress made in going from Eq. (1.6) to Eq. (1.1) for the finite potential case.

Having said all this by way of a brief historical survey, we may in retrospect consider the following points:

(i) The calculation leading to Eq. (1.1) can by no means be regarded as elementary, although the physical interpretation of the first term, at least, $2\pi N\rho a$, is obvious. It is simply the number of pairs of particles, $\frac{1}{2}N(N-1)$, times the ground energy of two particles, in a box of volume V. Yet to obtain this term one is obliged to sum an infinite series of graphs. There can be no doubt that some plain physics has been obscured by an overwhelming amount of difficult, albeit sophisticated, mathematics. The second term in Eq. (1.1), does not seem to have any very simple physical interpretation, and whatever meaning it does have is obscured by a twofold summation of an infinite series.

(ii) The mathematics itself is certainly not free from internal criticism. For one thing it was thought that one had isolated all the leading order terms when Eq. (1.6) was obtained; this did not prove to be the case. Can we be sure that we have now found all the appropriate terms in arriving at Eq. (1.1)? Secondly, for every term in the series leading to Eq. (1.1), it is easy to see that one has rejected an infinite number of terms each more

[3] L. Van Hove, Physica **18**, 145 (1952).
[4] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).
[5] N. M. Hugenholtz, Physica, **23**, 481 (1957).
[6] L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959).
[7] *The Many Body Problem*, edited by C. De Witt (John Wiley & Sons, Inc., New York, 1959), p. 343.
[8] K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1117 (1957).
[9] J. T. Beliaev, Zh. Eksperim. i Teor. Fiz. **34**, 417 (1958) [translation: Soviet Phys.—JETP **7**, 289 (1958)].
[10] N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).
[11] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).
[12] E. H. Lieb, Proc. Natl. Acad. Sci. U. S. **46**, 1000 (1960).

divergent than the one retained. Thirdly, the series leading to the second term of Eq. (1.6) diverges if one takes the correct order of limits $N\to\infty$ and *then* $\rho a^3\to 0$. This is because the series is a power series in $x=aN/L$, $(L^3=V)$, which, for dimensional reasons, must converge to $x^{5/2}$ for large x—clearly an impossibility. This difficulty was overcome by Lee, Huang, and Yang by a renormalization procedure at high energy; Bogoliubov relied on the fact that the high-momentum components of $v(\mathbf{x})$ went asymptotically to zero. But clearly high-momentum considerations should play no role for particles having very low energy, as in this problem.

(iii) The hard-core problem would seem to be a special case requiring extraordinary care. This is indeed strange in view of the fact that for the many-body problem, as for the elementary two-body problem, the hard-core potential is the only potential for which one can evaluate the potential energy *a priori* and show that it vanishes. All of E_0 is kinetic energy. Indeed one sees at once that the wave function vanishes whenever two or more particles overlap ($|x_i-x_j|\leq a$). Surely this very important piece of information, given *gratis* so to speak, must make the problem simpler rather than more difficult. A more direct and transparent solution of the problem must exist.

We should like to emphasize that we do not mean to be destructively critical or carping, nor to attempt to detract from the importance and usefulness of previous work. But there can be no harm in pointing out failings where they exist and to attempt to do something about them. In any case, if a complicated calculation can be made simpler and brought more into line with elementary notions it can be of benefit for future work. Finally, as in this case where the answer cannot be proved, a simpler derivation increases our confidence in the result.

We shall show how to obtain Eq. (1.1) by a straightforward method involving nothing more complicated than the mathematics of elementary quantum mechanics. [In a subsequent paper we shall discuss Eq. (1.2).] A hint that this is indeed possible is to be found in the fact that after Eq. (1.1) was found, it was shown that the same answer could be obtained variationally by a product trial function[13]

$$\phi=\prod_{\langle ij\rangle}[1+f(|\mathbf{x}_i-\mathbf{x}_j|)]. \tag{1.7}$$

The method to be given here is not approximate and is not a variational calculation. But we shall show that Eq. (1.1) can be obtained by a consistent and careful use of the superposition approximation familiar in classical statistical mechanics, which in the low-density limit is not an approximation at all but is asymptotically exact.

In an Appendix we shall briefly examine the *high*-density limit and among other things prove that Eq. (1.3) is asymptotically exact for a certain class of finite potentials.

II. SOME GENERAL CONSIDERATIONS

The Hamiltonian of the problem is

$$H=-\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2+\sum_{\langle i,j\rangle}v(|\mathbf{x}_i-\mathbf{x}_j|). \tag{2.1}$$

The first question that arises is what condition must we impose on v in order that the system in its ground state behave like a gas. By this is meant that there must not exist any many-body bound state or, more formally,

$$\lim_{\rho\to 0}E_0=0. \tag{2.2}$$

A necessary and sufficient condition for Eq. (2.2) is not known, but the following is easy to prove:

(i) Necessary conditions are that the scattering length of v be positive and that v does not have a two-body bound state;

(ii) A sufficient condition is that v be everywhere positive.

A necessary and sufficient condition lies somewhere between (i) and (ii) and we shall assume that for the potential in question, Eq. (2.2) is satisfied.

We shall further assume that v is of short range and that a length b exists such that

$$v(\mathbf{r})=0 \quad \text{for} \quad r\geq b. \tag{2.3}$$

Having thus described the problem, we now seek the ground-state energy, E_0, of H as a function of v and the density, in the case of low density. Before proceding to the mathematical analysis it is of central importance to have a clear idea of the relative sizes of the various lengths appearing in the problem.

It is to be assumed, although no one has ever proved this rigorously,[14] that in the limit $N\to\infty$, $V\to\infty$, $N/V=\rho$, E_0 is of the form

$$E_0=N\times\text{function of }\rho. \tag{2.4}$$

Unfortunately, ρ itself is not dimensionless and we must, therefore, look for a characteristic length in the problem. Without attempting to prejudice the issue we shall

[13] See, for example, J. B. Aviles Jr., Ann. Phys. (N.Y.) **5**, 251 (1958) [also, R. Jastrow, Phys. Rev. **98**, 1479 (1955)]. The author treats the hard-sphere problem and was able only to guess at the optimum form of f. This gave a result slightly greater than Eq. (1.1), but it has been subsequently shown [H. A. Bethe (private communication)] that a better choice for f gives exactly Eq. (1.1). K. Hiroike, [Progr. Theoret. Phys. (Kyoto) **27**, 342 (1962)] also derived Eq. (1.1) from a product function by using the hypernetted chain approximation.

[14] There is a heuristic proof of this, however, in O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956). For the hard-sphere case, F. J. Dyson [Phys. Rev. **106**, 20 (1957)] has effectively proved Eq. (2.4) by deriving rigorous upper and lower bounds for E_0 which are of the required form.

choose the scattering length, a, of v (alternatively b could be used). We may, therefore, write

$$E_0 = N\rho^{2/3} f(\rho a^3). \tag{2.5}$$

This is not to say that all potentials having the same scattering length give rise to the same energy, although this will indeed prove to be the case at low density. The point is, though, that for a given potential with $a>0$

$$\lim_{x\to 0} f(x) = 0, \tag{2.6}$$

a result which follows from examining the variational energy using ψ_0 as a trial function. If we assume that the energy is proportional to the number of pairs of particles at low density then

$$f(x) \sim x^{1/3}, \quad (x \text{ small}), \tag{2.7}$$

a result borne out by the variational calculation.

We may now consider three important lengths appearing in the problem. The first is $l_1 = a$ (or b), the second is $l_2 = \rho^{-1/3}$ (the average particle spacing), and the third is $l_3 = (\rho a)^{-1/2} = l_1^{-1/2} l_2^{3/2}$. As $\rho \to 0$, $l_1/l_2 \to 0$ and $l_2/l_3 \to 0$.

The significance of l_3 is that it is a kind of correlation length. If Eq. (2.2) is accepted, then

$$E_0 = Nk^2 \simeq N(l_3)^{-2}, \tag{2.8}$$

where k is the root mean square momentum per particle. Since E_0 is proportional to the number of pairs, k^{-1} or l_3 is thus seen to be of the order of the distance over which two particles are correlated, the distance being much greater than the average particle spacing. Clearly particles tend to decrease their momenta, this distance comes about from a chain of correlations via the intermediate neighbors. Because large distances are associated with low momenta, and because at low densities the particles tend to decrease their momenta, this distance increases with decreasing ρ. Put another way, we see that E_0 is entirely a quantum-mechanical correlation phenomenon; one cannot approximate ψ by a product of single-particle wave packets because either the potential energy would be too great (infinite for hard cores) if the size of a wave packet is larger than l_2 or, in the opposite case, the kinetic energy would be too great ($\sim N\rho^{2/3}$).

The situation here is vastly different from the corresponding Fermi gas at low density. There it is possible to think in terms of wave packets (at least to zeroth order)

$$f(x) = c_1 + c_2 x^{1/3}, \quad (x \text{ small, Fermi gas}) \tag{2.9}$$

where c_1 and c_2 are constants.

What can we learn from these considerations? The effect we are investigating is caused, so to speak, by a very small length, l_1. But it manifests itself at very large distances. The point is that although the potential is important, its effects at distances of the order of l_1, or even of l_2, is really unimportant. In the sequel, we shall work in configuration space and the analysis will consist in trying to evaluate the asymptotic behavior of certain correlation functions. This asymptotic behavior will then enable us to discover what we need to know about the correlation at distances of the order of l_1 in order to evaluate the energy.

III. CALCULATION OF THE GROUND-STATE ENERGY

We want to find the lowest state of H [see Eq. (2.1)] which is totally symmetric, but this is easily seen to be the absolutely lowest state of H (irrespective of symmetry). The absolutely lowest state of H satisfies

$$\psi \geq 0 \quad \text{for all} \quad \mathbf{x}_1, \cdots, \mathbf{x}_N, \tag{3.1}$$

a fact which can be proved by evaluating the variational energy of $|\psi|$. Equation (3.1) implies the important property

$$\int \cdots \int_V \psi(\mathbf{x}_1, \cdots, \mathbf{x}_N) \prod_{i=1}^{N} d^3x_i \equiv \int \psi > 0. \tag{3.2}$$

Since ψ is, therefore, not orthogonal to a totally symmetric function, viz., $f=1$, it must itself be totally symmetric, and, therefore, the contention above is proved. We have tacitly assumed that the ground state is nondegenerate, but this restriction is not necessary.[15,16]

[15] We have glossed over several points of a technical nature which we elucidate here. We do not assume, as other authors have done that the absolute (Boltzmann) ground state of H is nondegenerate. We first prove: (i) among the Boltzmann ground states there is at least one that satisfies $\psi \geq 0$. For a proof, we take the ground-state functions to be real and then take the absolute value of any one of them as a variational trial function. Since this does not change the energy, $|\psi|$ must also be a ground-state function. This device was used by Penrose and Onsager (reference 14) who claim to give the first proof that the Bose ground state is nonnegative. This device, however, ignores one difficulty, viz., does $|\psi|$ satisfy the boundary conditions? If the boundary conditions were that $\psi = 0$ on the boundary of the box, there would be no problem. But if ψ is periodic, $|\psi|$ will not have a periodic normal derivative if ψ happens to vanish on the boundary. We may overcome this difficulty, however, by the following artifice: If we use strict periodic boundary conditions (cf., reference 17), then we may regard the walls of the box as folded around onto each other (i.e., the square becomes a torus, the cube becomes a hypertorus). In applying the variational principle now, we require only continuity and piecewise differentiability of the wave function, and we do not have to require periodicity of the normal derivative. This latter property will be an automatic consequence of the Euler equations. We can now use $|\psi|$, and the proof of (i) goes through. If ψ is a positive Boltzmann function, then consider $\phi(\mathbf{x}) = \sum_P \psi(P\mathbf{x})$, where the summation is on all permutations. ϕ is clearly symmetric and does not vanish identically. In fact, it is non-negative because ψ is. It satisfies the Schrödinger equation and we, therefore, conclude: (ii) among the ground-state Boltzmann functions there is at least one non-negative Bose function. We now wish to prove: (iii) this non-negative Bose functions (call it ϕ) can be taken to have zero momentum. We need this fact in order to establish Eq. (3.6c) above. The proof is as follows: $\phi(\mathbf{x})$ can clearly be periodically extended so that it is defined over all space and satisfies the Schrödinger equation everywhere. By translational invariance of H, if $\phi(\mathbf{x})$ is an eigenfunction, then so is $\phi(\mathbf{x}+\mathbf{a})$ for arbitrary displacement $\mathbf{a}$ of all the particles. Define $h(\mathbf{x}) = \int_V \phi(\mathbf{x}+\mathbf{a}) d^3a$. The function $h(\mathbf{x})$ does not vanish and is non-negative since $\phi \geq 0$. Also h is a ground-state function and by explicit differentiation it has zero momentum. Q.E.D. We have

Let us integrate both sides of the equation

$$H\psi = E_0\psi. \tag{3.3}$$

It will be seen that for periodic boundary conditions the term $\frac{1}{2}\int(\sum \nabla^2)\psi$ vanishes and, using symmetry, we obtain

$$E_0 = \frac{N(N-1)}{2}\int v(|\mathbf{x}_1-\mathbf{x}_2|)\psi \Big/ \int\psi. \tag{3.4}$$

It will be appreciated that Eq. (3.2) was essential for obtaining Eq. (3.4).

We next define certain correlation or distribution functions which, unlike the customary definitions, are linear in ψ instead of being quadratic. That this is sensible is again a direct consequence of Eq. (3.1)

$$g^n(\mathbf{x}_1,\cdots,\mathbf{x}_n)$$

$$\equiv V^n\int\cdots\int_V \psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)\prod_{j=n+1}^{N} d^3x_j \Big/ \int\psi. \tag{3.5}$$

Periodic boundary conditions[17] imply that g^n is a periodic function of its arguments in V. Recalling the translational invariance of H, we have the following properties for the g^n:

$$g^1(\mathbf{x}_1) = \text{const} = 1, \tag{3.6a}$$

$$g^2 = g^2(\mathbf{x}_1-\mathbf{x}_2), \tag{3.6b}$$

$$g^n(\mathbf{x}_i+\mathbf{a}) = g^n(\mathbf{x}_i), \quad (\mathbf{a}=\text{arbitrary vector}), \tag{3.6c}$$

$$g^n \geq 0 \text{ all } \mathbf{x}_1, \cdots, \mathbf{x}_n, \tag{3.6d}$$

$$\int_V g^n(\mathbf{x}_1,\cdots,\mathbf{x}_n)d^3x_n = Vg^{n-1}(\mathbf{x}_1,\cdots\mathbf{x}_{n-1}). \tag{3.6e}$$

Finally, we need two more obvious facts which, unfortunately, must be assumed. Firstly, since $v(\mathbf{x})$ is a function of $|\mathbf{x}|$—if: (a) n is a fixed integer; (b) $\mathbf{x}_1, \cdots, \mathbf{x}_n$ are confined to a fixed region $R \subset V$; (c) V, and hence N, goes to infinity—then g^n is rotation invariant.

$$g^n(\mathbf{R}\mathbf{x}_i) = g^n(\mathbf{x}_i), \tag{3.6f}$$

where $\mathbf{R}$ is a rotation. In particular[18]

$$g(\mathbf{x}_1-\mathbf{x}_2) = g(|\mathbf{x}_1-\mathbf{x}_2|) = g(r), \quad \text{(large system)}. \tag{3.6g}$$

Equations (3.6f) and (3.6g) would seem to be implied by the principle of independence at large distances [cf. Eq. (3.13) below] but it is difficult to make this connection rigorous. The second property, namely,

$$\lim_{V\to\infty, N/V=\rho} g^n \equiv \tilde{g}^n, \text{ exists, } (n \text{ fixed}), \tag{3.6h}$$

means that we can speak of the correlation functions of a finite number of particles in the limit of a large system.[19] This property would appear to follow from Eq. (2.4), but here again a rigorous proof is difficult. Despite (3.6h), however, it will be necessary to some extent to consider the manner in which g^n approaches the limit. We shall return to this point later.

Returning to Eq. (3.4), it may be written

$$E_0 = \tfrac{1}{2}(N-1)\rho\int_V g(\mathbf{x})v(\mathbf{x})d^3x, \tag{3.7}$$

where we have purposely kept $N-1$ instead of N because we are not yet ready to pass to the limit of an infinite system. Equation (3.7) is our rigorous starting point for the calculation of E_0; it is clearly reminiscent of similar formulas in classical statistical mechanics.[20]

At this point we should consider the infinite repulsive core, for in this case Eq. (3.7) is meaningless as it stands. Taking the hard-sphere gas for simplicity, we have

$$-\tfrac{1}{2}\sum \nabla^2\psi = E_0\psi \text{ in } R, \tag{3.8a}$$

$$\psi \equiv 0 \text{ elsewhere and on boundary of } R, \tag{3.8b}$$

where the domain R is defined by

$$R\text{: all } |x_i-x_j| \geq a. \tag{3.9}$$

The wave function and its correlation functions still satisfy Eqs. (3.1), (3.2), (3.5), and (3.6), but now we can integrate Eq. (3.8a) only over R.

$$E_0 = -\tfrac{1}{2}N\int_R \nabla_1^2\psi \Big/ \int_V \psi. \tag{3.10}$$

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presented all this detail because the proofs in the literature are incomplete. Dyson (reference 14) quotes Yang to the effect that, since the Boltzmann ground state is non-negative and non-degenerate, all the above properties follow at once. The difficulty is that if the potential is sufficiently pathological there can be degeneracy. For hard spheres in one dimension, the Fermi and Bose ground states are degenerate if N is odd [cf., M. Girardeau, J. Math. Phys. **1**, 516 (1960)]. Indeed, if $\psi=0$ boundary conditions are used, then the ground states of all symmetry classes are degenerate for this problem [cf., E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962)]. Penrose and Onsager claim to prove that the Bose ground state is nondegenerate. This, too, is incorrect if the potential is sufficiently pathological. For a double hard-core potential in one dimension (i.e., $v(x)=\infty$ for $|x|<a$ and $b<|x|<c$, where $a<b<c$, $v(x)=0$ otherwise), for a certain value of L, the length of the box, there will be two degenerate ground-state Bose functions for two particles. Both of these functions may be taken non-negative; they are orthogonal, nevertheless, because when one is nonzero the other vanishes.

[16] Equation (3.2) is not true for the lowest Fermi function and, therefore, the subsequent analysis has to be modified if one wishes to apply it to the Fermi gas. In fact, one does not know *a priori* the spatial symmetry class of the lowest Fermi function, for the total spin need not be zero in the ground state as it is for the free-Fermi gas.

[17] Strict periodicity is implied, meaning that not only is ψ periodic but H as well. Strictly speaking, $v(\mathbf{x})$ must, therefore, be replaced by $\Sigma_{\mathbf{a}}\, v(\mathbf{x}+L\mathbf{a})$ where the summation is over all vectors, $\mathbf{a}$, whose components are integers, and where $V=L\times L\times L$.

[18] Henceforth, we shall use the symbol g in place of g^2.

[19] The same assumption is made in classical-statistical mechanics, and indeed is at the basis of any treatment of large systems.

[20] T. L. Hill, *Statistical Mechanics*, (McGraw-Hill Book Company, Inc., New York, 1956).

Integrating Eq. (3.10) by parts and using Eq. (3.8b) we obtain

$$E_0=\tfrac{1}{2}N(N-1)\int_V \prod_2^N d^3x_j \times\left\{\int_{r=a} a\mathbf{r}\cdot\nabla_1\psi(\mathbf{x}_2+\mathbf{r},\mathbf{x}_3\cdots\mathbf{x}_N)d\Omega_r\right\}\left(\int_V\psi\right)^{-1}$$
$$=2\pi(N-1)\rho a^2\frac{d}{dr}g(r)\,|_{r=a+} \tag{3.11}$$

upon using (3.6g). Thus,

$$4\pi\int_0^\infty g(r)v(r)r^2dr\to 4\pi a^2\frac{d}{dr}g(r)\,|_{r=a+} \tag{3.12}$$

for hard spheres. We remark in passing that

$$g^n=0 \text{ if any } |\mathbf{x}_i-\mathbf{x}_j|\leq a \quad \text{(hard spheres)} \tag{3.6i}$$

by virtue of Eq. (3.8b).

Hence, the hard-sphere case really requires no special treatment. Other integrals similar to Eq. (3.7) will arise and they can all be treated in the same way. We shall, therefore, continue to use these integrals in the hard-sphere case with the understanding that they can (rigorously) be replaced, as in Eq. (3.12), with meaningful expressions.

There is one more property of the correlation functions that needs to be mentioned, viz., the principle of independence at large distances (ILD). Taking g as an example, $\tilde{g}$ satisfies

$$\lim_{|\mathbf{x}|\to\infty}\tilde{g}(\mathbf{x})=\text{const}, \tag{3.13}$$

a fact which, while it cannot be proved,[21] is physically obvious. It means that the correlation between two particles disappears as they move apart. Using Eqs. (3.6a), (3.6b), and (3.6e) the constant in Eq. (3.13) is easily seen to be unity. By the same argument, all $\tilde{g}^n$ satisfy

$$\lim_{|\mathbf{x}_n|\to\infty}\tilde{g}^n(\mathbf{x}_1,\cdots,\mathbf{x}_n)=\tilde{g}^{n-1}(\mathbf{x}_1,\cdots,\mathbf{x}_{n-1}) \tag{3.14}$$

for fixed $\mathbf{x}_1$ through $\mathbf{x}_{n-1}$.

If we, therefore, write

$$\tilde{g}(\mathbf{x})=1-\tilde{u}(\mathbf{x}) \tag{3.15a}$$

and[22]

$$g(\mathbf{x})=\frac{1}{1-\delta}[1-u(\mathbf{x})]=(1+\delta)[1-u(\mathbf{x})]+o(V^{-1}), \tag{3.15b}$$

where

$$\delta=V^{-1}\int_V u(\mathbf{x})d^3x, \tag{3.15c}$$

then

$$\lim_{V\to\infty}u(\mathbf{x})=\tilde{u}(\mathbf{x}), \tag{3.15d}$$

and

$$\lim_{|\mathbf{x}|\to\infty}\tilde{u}(\mathbf{x})=0. \tag{3.15e}$$

The factor $(1-\delta)^{-1}$ in Eq. (3.15b) follows from Eq. (3.6e).

The next step is to find an equation for g. This may be done by operating on g with $-\frac{1}{2}(\nabla_1^2+\nabla_2^2)$ whence, using Eqs. (3.3) and (3.5), we obtain[23]

$$[-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)+v_{12}]g(1,2)=E_0g(1,2)-2V^{-1}(N-2)\times\int_V g^3(1,2,3)v_{23}d_3-\tfrac{1}{2}V^{-2}(N-2)(N-3)\times\int\int_V g^4(1,2,3,4)v_{34}d_3d_4\equiv M(1,2). \tag{3.16}$$

Let us consider the order of magnitude of the various terms appearing in Eq. (3.16). If V is very large, we may think of replacing g in the left-hand side by its limit function, which therefore makes the left-hand side of order unity in the volume (note that g^n is dimensionless). Of the three terms on the right-hand side, only the second is of order unity; the other two, being of order V (or N), must cancel each other to order V and leave a residue of order unity. That they indeed cancel may be seen in the following way: In the integrand of the third term we must have $|\mathbf{x}_3-\mathbf{x}_4|<b$, but otherwise the pair (3,4) can be anywhere. Clearly, the major contribution to the integral comes when (3,4) is far from either 1 or 2. In this region we may write $g^4(1,2,3,4)\simeq g(1,2)g(3,4)$ [in analogy with Eq. (3.14)]. Using Eq. (3.7), this contribution, when multiplied by the appropriate factor, yields $-E_0g(1,2)$. The correction, which is thus of order unity, comes from three sources: the presence of the factor $(N-2)(N-3)$ instead of $N(N-1)$; the contribution to the integral when (3,4) is close to either 1 or 2; and the fact that $g^4=\tilde{g}^4+$corrections of $O(V^{-1})$. In this context "close" means $\sim(\rho a)^{-1/2}$, the point being that for a fixed density and a very large system there must be some volume-independent distance beyond which the pairs (1,2) and (3,4) cease to be correlated.

For a large system the function $M(1,2)$ is volume-independent but it is also clear that is essentially proportionally to e, the energy per particle;

$$e=N^{-1}E_0. \tag{3.17}$$

We may, therefore, assume that if we consider ρ to be very small and define

$$G(r)\equiv\lim_{\rho\to 0}\tilde{g}(r), \tag{3.18}$$

[21] O. Penrose and L. Onsager, (reference 14) almost succeeded in proving ILD.

[22] $o(x)$ means the quantity in question is of *lower* order than x. $O(x)$ means the same order as x.

[23] In Eq. (3.16) *et seq.* we use the standard notation of statistical mechanics, Cf. reference 20. $g_{12}\equiv g(1,2)\equiv g(\mathbf{x}_1,\mathbf{x}_2)$; $\int d_1\equiv\int d^3x_1$.

then

$$[-\nabla^2+v(\mathbf{x})]G(\mathbf{x})=0. \tag{3.19}$$

This means that in the limit of zero density g is the solution to the zero-energy scattering problem with the potential $v(\mathbf{x})$, a physically satisfying situation. Inserting G into Eq. (3.7) we obtain the result

$$E_0=2\pi N\rho a+o(\rho), \tag{3.20}$$

where a is the scattering length, in agreement with Eq. (1.1). Thus, without further ado, and certainly without summing an infinite set of graphs, we have obtained the leading term in the energy.

For the hard-sphere case we have

$$\begin{aligned} G(r)&=1-a/r, \quad r>a \\ &=0, \qquad r<a. \end{aligned} \tag{3.21}$$

It will be noticed that $G(r)$ has no cutoff length. Physically, the reason is that the cutoff length, $(\rho a)^{-1/2}$, becomes infinite for zero density. Mathematically speaking, the convergence in Eq. (3.18) is nonuniform. To orient ourselves, we may suppose that $\tilde{g}(r)=1-(a/r)\times\exp[-(\rho a)^{1/2}(r-a)]$, a function that has been used in variational calculations.[13] Its limit at zero density is given by Eq. (3.21).

To make further progress, we must attempt to evaluate $M(r)$, and the crucial point here is that we need to know it only for large distances—of the order of $(\rho a)^{-1/2}$. Taking the hard-sphere gas as an example, we have from Eqs. (3.12) and (3.16)

$$e=2\pi\rho a\left(1+\int_a^\infty rM(r)dr\right). \tag{3.22}$$

Thus, if $u(r)$ and hence $rM(r)$ have a certain large cutoff length, l, the major contribution to the integral in Eq. (3.22) will come from distances of the order of l. But at the same time, whatever l may be, it is the distance at which Eq. (3.14) begins to be true.

For the first integral in Eq. (3.16) we see that we need to know $g^3(1,2,3)$ when 2 and 3 are close together and 1 is far removed, by a distance of order l. It seems quite obvious, although we cannot prove it, that in this asymptotic region g^3 may be written

$$g^3(1,2,3)=s[1-w(1,2)][1-w(1,3)][1-w(2.3)], \tag{3.23}$$

where s is a positive constant. If

$$\lim_{V\to\infty} w(\mathbf{x})=\tilde{u}(\mathbf{x}) \quad \text{and} \quad \lim_{V\to\infty} s=1, \tag{3.24}$$

then the assumption, (3.23), is consistent with Eqs. (3.6) and (3.14). But for a finite system we do *not* suppose that $w=u$ for we shall be interested in the difference between w and u which is $o(1)$ in the volume. To determine s and w we use Eq. (3.6e), which is consistent, for although we must integrate x_3 over all space the major contribution to the integral in (3.6e) comes from the asymptotic region where Eq. (3.23) is presumably correct. One easily finds that

$$s=1+3\delta+o(\delta), \tag{3.25}$$

$$w(1,2)=u(1,2)+\frac{1}{V}g(1,2)\int_V u(1,3)u(2,3)d_3+o(\delta). \tag{3.25b}$$

Actually, the V^{-1} corrections to s and w given by Eq. (3.25) will play no role when we evaluate the first integral in Eq. (3.16), for that term is already of order unity in the volume. We obtain (upon passing to the limit of an infinite system)

$$\int_V g^3(1,2,3)v_{23}d_3 \cong g(1,2)\left[\frac{2e}{\rho}-\int_V u(1,3)g(2,3)v_{23}d_3\right], \tag{3.26}$$

where limiting functions and integrals are understood on the right-hand side of Eq. (3.26). We repeat the assertion that Eq. (3.26) is asymptotically correct for large $|\mathbf{x}_1-\mathbf{x}_2|$ and small ρ, and that this is just what is needed in Eq. (3.16) to get the second term in E_0 as a function of ρ.

When we turn to the second integral, however, and apply the same arguments, V^{-1} corrections will be decidedly important. If we write

$$g^4(1,2,3,4)\to t\prod_{\langle i,j\rangle}[1-h(i,j)] \tag{3.27}$$

and use Eq. (3.6e) twice,[24] we obtain

$$t=1+6\delta+o(\delta), \tag{3.28a}$$

$$h(1,2)=u(1,2)+\frac{2}{V}g(1,2)\int_V u(1,3)u(2,3)d_3+o(\delta). \tag{3.28b}$$

If we now insert Eqs. (3.28) and (3.26) into Eq. (3.16) and combine terms, we get the final equation for g:

$$[-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)+v_{12}]g(1,2)=\rho g(1,2)\{2K(1,2)-\rho L(1,2)\}, \tag{3.29}$$

where

$$K(1,2)=\int_V u(1,3)g(2,3)v_{23}d_3 \tag{3.30a}$$

and

$$L(1,2)=\int\int_V u(1,3)u(2,4)\{g(1,4)g(2,3)-\tfrac{1}{2}u(1,4)u(2,3)\}\times g(3,4)v(3,4)d_3d_4. \tag{3.30b}$$

[24] Unfortunately, if we insert Eq. (3.27) into (3.6e) we will not obtain Eq. (3.23) for, if we did, it would mean that the product *ansatz* would be exact. The best we can do, therefore, is to make g^4 consistent with g.

Furthermore, since Eq. (3.29) is valid only when $|\mathbf{x}_1-\mathbf{x}_2|\gg b$ we can clearly replace the factors $g(2,3)v_{23}$ and $g(3,4)v_{34}$ appearing in Eq. (3.30) by their average value, viz., $\frac{1}{2}e\rho^{-1}$. It might be supposed that we could now replace u and g on the right-hand side of Eq. (3.29) by their zero-density limit [Eq. (3.19)], but this would lead to a divergent integral in Eq. (3.30b). This integral converges, however, because u has a cutoff length. On the other hand, there is no harm in replacing the terms in the parenthesis in Eq. (3.30b) by their zero-density limit. But we can go further than this and replace the entire parenthesis by unity because for the range of $\mathbf{x}_1-\mathbf{x}_2$ in which we are interested, u can be neglected compared to one. This is clear from Eq. (3.21) or (3.19), where we see that up to the cutoff, $u(r)$ is essentially proportional to r^{-1}. In the same spirit, we can replace the factor $g(1,2)$ on the right-hand side of Eq. (3.29) by unity.

Having thus "linearized" Eqs. (3.29) and (3.30), Eq. (3.29) becomes

$$[-\nabla^2+v(r)][1-u(r)]$$
$$=4eu(r)-2e\rho\int_V u(\mathbf{r}-\mathbf{z})u(\mathbf{z})d^3z, \quad (3.31)$$

the last term being clearly a function of $r=|\mathbf{r}|$. It must be emphasized that the linearization of Eq. (3.29) leading to Eq. (3.31) did not alter the long-range part of $M(r)$—at least to leading order in ρ—and that the solution of Eq. (3.31), therefore, will give the next higher term in the energy exactly when it is inserted into Eq. (3.7). But since Eq. (3.31) contains e as a parameter, Eq. (3.7) will become an algebraic equation for e.

Were it not for the presence of $v(r)$, Eq. (3.31) could be solved exactly by a Fourier transformation, because the integral is in the form of a convolution. Nevertheless, since we are only interested in the right-hand side for $r\gg a$, a Fourier transform may still be used to advantage. Taking transforms of both side of Eq. (3.31) we have

$$-k^2u(k)+(2e/\rho)S(k)=4eu(k)-2e\rho u^2(k), \quad (3.32)$$

where

$$u(k)=\int u(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}d^3r \quad (3.33a)$$

and

$$S(k)=\frac{\rho}{2e}\int g(\mathbf{r})v(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}d^3r. \quad (3.33b)$$

The solution to Eq. (3.32) is

$$\rho u(k)=(x^2+1)-[x^4+2x^2+1-S(k)]^{1/2}$$
$$\sim\tfrac{1}{2}S(k)[x^{-2}-x^{-4}+O(x^{-6})], \quad \text{large } k, \quad (3.34)$$

where

$$4ex^2=k^2. \quad (3.35)$$

We now write

$$u=u_1+u_2, \quad (3.36)$$

where

$$\rho u_1(k)=(2e/k^2)S(k). \quad (3.37)$$

Since

$$u(r)=\frac{1}{2\pi^2}\int_0^\infty k^2dk\,u(k)\frac{\sin kr}{kr}, \quad (3.38)$$

we see that $u_1(r)$ is the solution to the equation

$$-\nabla^2u_1(\mathbf{x})=g(\mathbf{x})v(\mathbf{x}), \quad (3.39)$$

which means that

$$u_1(r)=(e/2\pi\rho)(1/r), \quad r\geq b, \quad (3.40)$$

by Gauss' theorem and Eq. (3.7).

Now because $S(k)\to 0$, as $k\to\infty$, and since $u_1(k)$ is just the asymptotic part of $u(k)$,we see that $u_2(k)$ vanishes at least like k^{-4} for large k. Furthermore, $S(k=0)=1$, and $S(k)$ will not depart from unity until k is of the order of b^{-1}, at which point $k^2u_2(k)$ is negligible. Therefore, to the order in which we are interested

$$u_2(r)=4\frac{e^{3/2}}{\pi^2\rho}\int_0^\infty dx\,x^2\frac{\sin\lambda xr}{\lambda xr}$$
$$\times\left(x^2+1-x(x^2+2)^{1/2}-\frac{1}{2x^2}\right), \quad (3.41)$$

where $\lambda=2\sqrt{e}$. It will be seen that for r of the order of b or less, $u_2(r)$ is a very slowly varying function and, for the accuracy we need, it may be replaced by its value at $r=0$. Later on we shall discuss the function defined by Eq. (3.41), but for the present, it is an elementary exercise to deduce that

$$u_2(0)=-\frac{32\sqrt{2}}{15\pi^2\rho}e^{3/2}\approx-\frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}, \quad (3.42)$$

the last expression being obtained by replacing e by its leading term [Eq. (3.20)].

The essential point to notice is this: As we see from Eq. (3.19), for small values of r the function g(or u) oscillates, and this oscillation is contained almost entirely in u_1. Since $g=1-u_1-u_2$

$$-\nabla^2g\approx\nabla^2u_1 \quad (3.43)$$

and hence, from Eq. (3.39),

$$-\nabla^2g+vg=0 \quad \text{for} \quad r\lesssim\rho^{-1/3}. \quad (3.44)$$

Equation (3.44) tells us that for small r, g is proportional to G, the first approximation to g, and is, therefore, very sensitive to the details of $v(r)$. But for large r, g is very different, being given by two universal functions, u_1 and u_2, which contain the energy as their only parameter. Thus,

$$g(r)=AG(r) \quad \text{for} \quad r\lesssim\rho^{-1/3}, \quad (3.45a)$$

where A is some constant, and

$$g(r)=A(1-a/r) \quad \text{for} \quad b\leq r\lesssim\rho^{-1/3}, \tag{3.45b}$$

$$=1-u_2(r)-u_1(r)\approx 1-u_2(0)-e/2\pi\rho r. \tag{3.45c}$$

Equating coefficients in Eq. (3.45), we obtain

$$A=1-u_2(0) \tag{3.46a}$$

and

$$e/2\pi\rho a=A. \tag{3.46b}$$

Thus,

$$e=2\pi\rho a\{1+(128/15\sqrt{\pi})(\rho a^3)^{1/2}+o[(\rho a^3)^{1/2}]\}, \tag{3.47}$$

in conformity with Eq. (1.1). We have thus, established that the first correction to e depends only upon the scattering length of v; higher corrections will clearly involve the effective range.[25] It is tempting, however, to solve Eq. (3.46) exactly. That is,

$$e/2\pi\rho a=1-u_2(0)=1+(32\sqrt{2}/15\pi^2\rho)e^{3/2}. \tag{3.48}$$

This is a cubic equation whose positive root has the correct general behavior up to $e=6\pi\rho a$, $\rho a^3=(\pi/3)(5/64)^2$, and then becomes complex. This value of ρa^3 is only about $\frac{1}{2}\%$ of the value at tight packing, viz., $\sqrt{2}$. In order to make any further progress it would be necessary to go back to Eq. (3.29)—clearly a job for machine computation. We can, however, learn something from Eq. (3.48). For the range of density over which it makes sense, it probably gives a better approximation for e than the first two terms in the asymptotic series, (3.47). At the limiting density mentioned above, it gives $e=6\pi\rho a$ while (3.47) gives $e=2\pi\rho a(1+2/3\sqrt{3})$. We may thus conclude that the $e(\rho)$ curve rises much more sharply than (3.47) would indicate, and that (3.47) is probably numerically accurate only for a much smaller density than the above limiting density.

We now return to the evaluation of $u_2(r)$ [Eq. (3.41)], that part of u which depnds only upon the scattering length. We define

$$R=(8e)^{1/2}r\approx 4(\pi\rho a)^{1/2}r \tag{3.49a}$$

and

$$u_2(r)=\frac{8e}{\pi^2\rho r}f(R)\approx\frac{16a}{\pi r}f(R). \tag{3.49a}$$

The integral in Eq. (3.41) may be transformed into a contour integral around the cut $(\sqrt{2}i-\sqrt{2}i)$ with the result that

$$f(R)=\int_0^1 dz\, z^2(1-z^2)^{1/2}(e^{-Rz}-1). \tag{3.50}$$

[25] It is clear how one could get higher corrections to Eq. (1.1) using the formalism presented here. One can derive an equation for g^3 and g^4 in analogy with (3.16) and solve them using superposition. Then insert the results into Eq. (3.16) and solve for a new $g(1,2)$. On the other hand, as Eq. (3.48) *et seq.* shows, such an asymptotic expansion is probably of academic interest only. A much better thing to try to do is to solve the full nonlinear equation, (3.29).

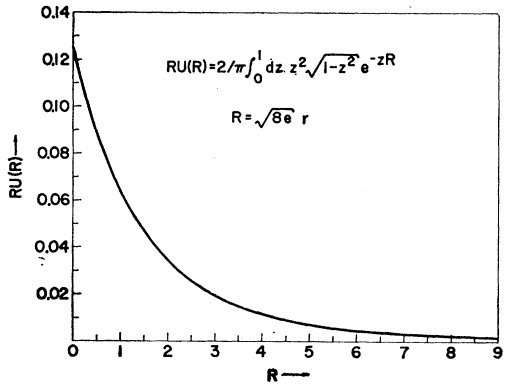

FIG. 1. The universal part of the two-particle correlation function, $g(r)\equiv 1-u(r)$, is given by $u(r)=[4(2e)^{3/2}/\pi\rho]U(R)$ $\approx 32(\pi\rho)^{1/2}a^{3/2}U(R)$. The ground-state energy per particle is $e\approx 2\pi\rho a$, and the dimensionless variable R is given by $R=(8e)^{1/2}r\approx 4(\pi\rho a)^{1/2}r$. This definition of $u(r)$ is valid for $r>b$, where b is the distance beyond which the two-body potential vanishes. $b\ll\rho^{-1/3}\ll(\rho a)^{-1/2}$. For $0<r<b$, $g(r)$ is the zero-energy scattering function of the potential.

It is elementary to deduce that, for small R,

$$f(R)=-(2/15)R+O(R^2), \tag{3.51}$$

which, when combined with Eq. (3.49), gives Eq. (3.42). It is also elementary to integrate the second term in parenthesis in Eq. (3.50). This yields a constant of course which, when combined with Eq. (3.49), gives $-e(2\pi\rho r)^{-1}$. But this is just the value of $-u_1(r)$ for $r\geq b$. Hence, for $r\geq b$

$$u(r)=\frac{8e}{\pi^2\rho r}\int_0^1 dz\, z^2(1-z^2)^{1/2}e^{-Rz} \tag{3.52}$$

$$\equiv(4/\pi\rho)(2e)^{3/2}U(R).$$

Equation (3.52) is not valid for $r<b$—it goes like R^{-1} and this is incorrect. Instead, Eq. (3.44) defines u for $r\lesssim b$. Equation (3.46) insures that in the overlap region $(b\leq r\lesssim\rho^{-1/3})$, these two definitions of $u(r)$ are substantially the same. Furthermore, the effective cutoff length of $u(r)$ is seen to be of the order of $l_3=(\rho a)^{-1/2}$, in agreement with Sec. II.

The integral in Eq. (3.52) can be evaluated in terms of Bessel functions. The result is:

$$U(R)=R^{-3}\{R[I_1(R)-L_1(R)] -3[I_2(R)-L_2(R)]\}, \tag{3.53}$$

where $L(R)$ is the modified Struve function and $I(R)$ is the modified Bessel function of the first kind.[26] Both $I(R)$ and $L(R)$ go to ∞ as $R\to\infty$, but their difference is finite. When R is large, $U(R)\sim R^{-4}$—a result found previously by Lee, Huang, and Yang in the hard-sphere case.[11] The function $U(R)$ is plotted in Fig. 1.

[26] A. Erdelyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 38; *Tables of Integral Transforms*, edited by A. Erdelyi (McGraw-Hill Book Company, Inc., New York, 1954), Vol. I, p. 138, No. 12.

APPENDIX

The High-Density Limit

While Bogoliubov's result, Eq. (1.3), is never correct at low density because it replaces the scattering length, a, by a', the first Born approximation to a, we wish to show here that it is correct in the limit of high density for a certain class of finite potentials. The discussion presented here is independent of the previous results of this paper, but it is interesting in that it shows that Bogoliubov's original point of view, which seems at first sight very reasonable, is really a high-density *ansatz*.

The basic idea behind Bogoliubov's theory is that in some sense the interacting particles behave like free particles to a first approximation. Although at low density $\psi \simeq \psi_0$ when the particles are far apart, as we have seen the important region to consider is when two particles are close together. In this latter region ψ is different from ψ_0 and the difference does not vanish as $\rho \to 0$.

Let us now inquire what happens as the density gets very large. For a potential with a hard core one can only go up to the critical density, $\rho_c a^3 = \sqrt{2}$, at which point the ground-state energy, E_0, becomes infinite. For a finite potential, on the other hand, as we go to high density (such that $\rho b^3 \gg 1$, where b = range of the potential) basically one of two things can happen:

(i) Some definite type of particle configuration (presumably a lattice) may be preferred. In this case, the particles will become localized with respect to each other (i.e., particle correlations will become important) and the kinetic energy will increase with density and become quite large, possibly unbounded. The large kinetic energy will be compensated by the favorable potential energy of the configuration. Such a situation presumably occurs in the hard-core case shortly before reaching the critical density.

(ii) No special configuration is preferred because the advantage of a low potential energy configuration is outweighed by the high kinetic energy required to achieve it. In this case the particles are "smeared" and the kinetic energy goes to zero as $\rho \to \infty$. Owing to the high density, each particle "sees" a constant potential—the average potential of its many neighbors. It is in this case that we may think of the wave function as approximately the noninteracting wave function, ψ_0, because correlations become less important as the density increases. For this case to hold it is not essential that the potential be everywhere repulsive. As we shall see, it can even have a two-body bound state.

We shall show here that there is a class of potentials for which case (ii) holds, and for which Bogoliubov's theory is then valid—at least for the ground-state energy. Let $v(\mathbf{r})$ be the two-body potential, and $\nu(\mathbf{k})$ be its Fourier transform defined by

$$\nu(\mathbf{k}) = \int v(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3r. \tag{A1}$$

The potentials we wish to consider satisfy

$$v(0) = \alpha = \text{finite}, \tag{A2a}$$

$$\nu(\mathbf{k}) \geq 0, \text{ all } \mathbf{k}. \tag{A2b}$$

A repulsive Gaussian potential, for example, is of this class. Notice that we do not assume $v(\mathbf{r}) > 0$, or even that the scattering length is positive. Consider the potential which is a repulsive square well in momentum space:

$$\begin{aligned} \nu(\mathbf{k}) &= \lambda, \quad k < K \\ &= 0, \quad k > K, \end{aligned} \tag{A3a}$$

$$v(\mathbf{r}) = -\lambda (K/2\pi^2 r^2)[\cos rK - (1/rK)\sin rK], \tag{A3b}$$

where λ and K are positive constants. This potential can have a two-body bound state if λ is sufficiently large, yet it is in our class.

We propose to find an upper and lower bound for the ground-state energy. An upper bound is obtained from the variational principle using $\psi_0 = 1$, viz.,

$$e < \tfrac{1}{2}\rho\nu(0), \tag{A4}$$

where $E_0 = Ne$. For the lower bound we use the fact that the kinetic energy is positive definite, whence

$$e > N^{-1} \min_{(\mathbf{x}_1, \cdots, \mathbf{x}_N)} \sum_{\langle i,j \rangle} v_{ij} \equiv B. \tag{A5}$$

Equation (A5) states that $E_0 >$ minimum potential energy. Let the minimum configuration occur at $\mathbf{x}_i = \mathbf{a}_i$. Then

$$B = \min_{\{\mathbf{a}_i\}} \frac{1}{2N} \int\int \phi^*(\mathbf{x}) v(x-y) \phi(\mathbf{y}) d^3x d^3y - \tfrac{1}{2}\alpha, \tag{A6}$$

where

$$\phi(\mathbf{x}) = \sum_i \delta(\mathbf{x} - \mathbf{a}_i). \tag{A7}$$

If $\tilde{\phi}(\mathbf{k})$ is the Fourier transform of $\phi(\mathbf{x})$, [cf., Eq. (A1)], then

$$B = (2NV)^{-1} \sum_{\mathbf{k}} |\tilde{\phi}(\mathbf{k})|^2 \nu(\mathbf{k}) - \tfrac{1}{2}\alpha \tag{A8a}$$

$$> \tfrac{1}{2}\rho\nu(0) - \tfrac{1}{2}\alpha, \tag{A8b}$$

where the last inequality follows from (A2b) and the fact that $\tilde{\phi}(0) = N$, whatever $\{\mathbf{a}\}$ may be. Thus, combining (A4) and (A8),

$$\tfrac{1}{2}\rho\nu(0) > e > \tfrac{1}{2}\rho\nu(0) - \tfrac{1}{2}\alpha, \text{ (all } \rho), \tag{A9}$$

Since α = finite, we have proved that the asymptotic form of e is $\frac{1}{2}\rho\nu(0)$. Moreover, with upper/lower bound

formulas for expectation values,[27] it is an easy matter, using the above inequalities, to prove that

$$t<\tfrac{1}{2}\alpha \quad (\text{all } \rho),$$
$$\tfrac{1}{2}\rho v(0)>v>\tfrac{1}{2}\rho v(0)-\tfrac{1}{2}\alpha \quad (\text{all } \rho), \tag{A10}$$

where t is the kinetic energy and v the potential energy per particle. Equation (A10) establishes that the kinetic energy remains bounded at high density. Actually, using a better upper bound than (A4), we shall show that for large ρ

$$t=o(\rho^{-\epsilon}), \tag{A11a}$$
$$v=\tfrac{1}{2}\rho v(0)-\tfrac{1}{2}\alpha+o(\rho^{-\epsilon}), \tag{A11b}$$
$$e=\tfrac{1}{2}\rho v(0)-\tfrac{1}{2}\alpha+o(\rho^{-\epsilon}), \tag{A11c}$$

where $\epsilon=$positive constant.

Equation (A11b) is a bit surprising in that we have proved that $\frac{1}{2}\rho v(0)-\frac{1}{2}\alpha$ is actually less than the minimum potential energy. The explanation is as follows: From the fact that $t\to 0$, we see that the minimum potential energy is not very different from the potential energy in a perfectly smeared wave function, i.e., $\psi_0=1$. In this case, the potential seen by a test charge would be $\rho v(0)$. The potential seen by one of the particles of the gas itself would be $\rho v(0)-\alpha$, because α is the effect of a particle on itself. Finally, dividing by two because we have double counted, we obtain the expression (A8b) for B. In other words, as regards the value of B itself, (A8b), in fact, gives correctly the first two terms in an asymptotic series for B in terms of ρ. On the other hand, from the fact that (A8b) was obtained without explicit reference to the minimum potential configuration $\{\mathbf{a}\}$, we see that the potential has an exceedingly broad minimum which in the limit of high density may be taken to be virtually the entire configuration space. This leads in turn to the result that $\lim_{\rho\to\infty} t=0$.

To obtain an improvement on (A4), and thereby establish Eqs. (A11), we turn to the variational calculation of Girardeau.[28] Following the notation of that paper, we see that if we choose $\phi(\mathbf{k})=1$ and set $\rho_0=\rho$ the integrals involving $v(\mathbf{k})$ would give us exactly $-\frac{1}{2}\alpha$. We cannot do this, however, for two reasons: The integrals involving k^2, I_1, and I_2, all of which are positive, would diverge; and $\rho-\rho_0$ would also diverge. But by choosing $\phi(\mathbf{k})=1-\rho^{-\alpha}f(k)$, for a suitable choice of α and $f(k)$ we can obtain an upper bound for e of the form of the right-hand side of Eq. (A11c). We omit the details here. Combining the result with (A9) we thus prove Eqs. (A11).

We turn now to the predictions of Bogoliubov's theory.[7] One has $e=e'+e''$, where

$$e'=\tfrac{1}{2}\rho v(0), \tag{A12a}$$

$$e''=(16\pi^3\rho)^{-1}\int d^3k \times\{\tfrac{1}{2}k[k^2+4\rho v(\mathbf{k})]^{1/2}-\tfrac{1}{2}k^2-\rho v(\mathbf{k})\}. \tag{A12b}$$

In the low-density limit we obtain Eq. (1.6) for any potential such that $v(\mathbf{k})/k^2$ is integrable. Lee, Huang, and Yang[11] were the first to obtain the famous factor $128/15\sqrt{\pi}$, but this factor is already implicit in Eq. (A12) which antedates their work.

For high density, the major contribution to e'' comes from the last term in the integrand and the total result is in agreement with (A11c). It is to be noted that both in Eq. (A11c) and in Eq. (A12b) the correction of $o(\rho^{-\epsilon})$ is positive.

[27] E. H. Lieb and K. Yamazaki, Phys. Rev. **111**, 728 (1958).

[28] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959), Eqs. (20)–(22).