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Quantum-Mechanical Many-Body Problem with Hard-Sphere Interaction

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The system under consideration is an N-particle quantum-mechanical system enclosed in a volume V, in which the particles interact via two-body hard-sphere potentials, with hard-sphere diameter a. The two-body hard-sphere problem is first discussed by a generalization of Fermi's pseudopotential by means of which the problem is formulated entirely in terms of the scattering phase shifts. It is then shown that a pseudopotential for the N-body problem can be introduced, and leads to an expansion of the energy levels of the system in powers of a. The first order energy levels of a Bose and a Fermi system are calculated. For the Bose system, the first order energy formula exhibits an "energy gap" above the ground state, leading to properties of the system not dissimilar to that of a superfluid. The ground state energy for a Bose system is calculated to order a^3 and that for the Fermi system, to order a^2. The physical interpretation and validity of these results are discussed.

1. INTRODUCTION

THE aim of the present investigation is to formulate the quantum-mechanical many-body problem in terms of the solution of the two-body problem.[1] In particular, at low energies, the purpose is to formulate the problem in terms only of the low-energy parameters of the phase shifts, e.g., scattering length, effective range, etc. The general program is to make expansions in powers of these parameters and to determine the region of validity of such expansions.

It is physically obvious that a complete knowledge of the detailed interaction potential is often not necessary for a satisfactory description of the system. For example, when a state of the many-body system is such that the particles are so far apart from one another that their fields of force do not appreciably overlap, their mutual influence is essentially determined by the asymptotic wave functions, which are directly related to the phase shifts. Furthermore, under certain conditions only a few phase shifts are important. For example, at low energies, all but the S-wave phase shift are negligible. The proposed formulation would provide a natural framework in which an approximation such as this could be systematically carried out.

Our formulation will be made for the special case of N particles with hard-sphere interactions. This will make the discussion concrete and help to make the physical picture more easily visualized. There is in fact little loss of generality in considering this special case as it embodies the main difficulty of the many-body problem. If this particular example is understood, it would not be difficult to extend the method to a more general case.

The general method we follow is to replace the interaction between the particles by suitable boundary conditions. Such methods have been discussed by various people.[2] In particular, Fermi,[3] Breit,[4] and Blatt and Weisskopf[5] have introduced a "pseudopotential" as an equivalent of the boundary condition. The use of this pseudopotential has always been confined to the Born approximation in scattering problems. We shall prove that for the two-body system a suitably generalized pseudopotential can be found that gives exact results. It will be demonstrated further that for the many-body problem the corresponding pseudopotential has a simple physical meaning which suggests a systematic approximation procedure.

The application of this procedure to the N-body hard-sphere problem results in expansions of the eigenvalues and eigenfunctions of the system in powers of the hard-sphere diameter a. The ground state energy for the Bose system is carried out to order a^3, and that for the Fermi system to order a^2. *For a finite number of particles, these expansions become meaningful for sufficiently large volumes.* To the orders specified they are exact. The method can therefore be applied to obtain series expansions of the equations of state for a Bose or a Fermi imperfect gas with hard-sphere interactions. We shall return to this in a subsequent paper.

2. TWO-BODY PROBLEM

(a) Formulation of the Pseudopotential in the Two-Body System

We shall first formulate the two-body problem in terms of a pseudopotential. As stated in the introduction, we consider the special case of a system of two particles with hard-sphere interaction. The wave function in the center-of-mass coordinate system then satisfies the equations

$$\begin{aligned}(\nabla^2+k^2)\psi(\mathbf{r})&=0, \quad (r>a)\\ \psi(\mathbf{r})&=0, \quad (r\leq a)\end{aligned} \tag{1}$$

where a is the hard-sphere diameter, $r=|\mathbf{r}|$, with $\mathbf{r}$ the relative position vector. The boundary condition at

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[1] Somewhat similar ideas have been discussed by Brueckner in his work on the nuclear problem. See K. A. Brueckner and W. Wada, Phys. Rev. **103**, 1008 (1956) and papers referred thereto.

[2] This idea appears to be first discussed by E. P. Wigner, Phys. Rev. **83**, 253 (1933).

[3] E. Fermi, Ricerca sci. **7**, 13 (1936).

[4] G. Breit, Phys. Rev. **71**, 215 (1947).

[5] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952), p. 74.

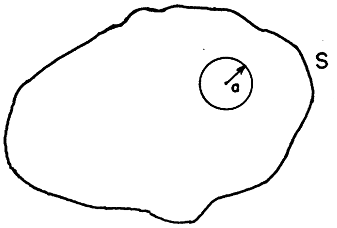

FIG. 1. Boundary conditions for two-body hard-sphere problem: $\psi(\mathbf{r})=0$ when $\mathbf{r}$ is on some distant surface S, and $\psi(\mathbf{r})=0$, when $r=a$.

infinity is, for example, that $\psi(\mathbf{r})=0$ for $\mathbf{r}$ on some arbitrary surface S (see Fig. 1).

For orientation, let us first discuss the S-wave part of the solution. As is well known, the S-wave phase shift for this case is

$$\eta_0=-ka. \tag{2}$$

We recognize that the hard-sphere diameter a can also be looked upon as the scattering length. According to Blatt and Weisskopf,[4] one can extend the wave function into the region $r<a$ such that

$$(\nabla^2+k^2)\psi(\mathbf{r})=4\pi a\delta(\mathbf{r})\frac{\partial}{\partial r}(r\psi), \tag{3}$$

where the operator operating on ψ on the right-hand side of (3) is known as the pseudopotential.

We now proceed to give a derivation of a generalized pseudopotential, which would *exactly* replace the hard-sphere potential for all partial waves and at all energies. Equation (3) is inexact for two reasons: First, it has not taken into account the higher partial waves, and secondly, even for S waves, it is valid only for very low energies since it has not included the S-wave parameters beyond the scattering length, such as the effective range.

We make an expansion of the wave function in spherical harmonics immediately outside the sphere $r=a$:

$$\psi(\mathbf{r})=\sum_{l,m} A_{lm}[j_l(kr)-(\tan\eta_l)n_l(kr)]Y_{lm}(\Omega), \tag{4}$$

where $Y_{lm}(\Omega)$ is a normalized spherical harmonic, and j_l, n_l, are the usual spherical Bessel functions. A_{lm} are constants which depend on the boundary condition on S, and the constants $\tan\eta_l$ are given by

$$\tan\eta_l=j_l(ka)/n_l(ka), \tag{5}$$

as required by the boundary condition $\psi(a)=0$. We see that η_l is no other than the phase shift of the lth partial wave. We would like to find the wave equation satisfied by $\psi(\mathbf{r})$ of (4), in such a way that the constants A_{lm} do not explicitly occur. First define

$$\psi_{lm}(r)=\int\psi(\mathbf{r})Y_{lm}{}^*(\Omega)d\Omega. \tag{6}$$

We see that for $r\geqslant a$,

$$\psi_{lm}(r)=A_{lm}[j_l(kr)-(\tan\eta_l)n_l(kr)]. \tag{7}$$

This last equation serves also to define ψ_{lm} inside the sphere $r=a$. Near the origin $r=0$, we make use of the well-known expansions for the spherical Bessel functions j_l and n_l:

$$j_l(kr)\xrightarrow[r\to0]{}(kr)^l/(2l+1)!!,$$

$$n_l(kr)\xrightarrow[r\to0]{}-(2l-1)!!/(kr)^{l+1},$$

where

$$(2l+1)!!=1\cdot3\cdot5\cdots(2l+1).$$

We can now write

$$\psi_{lm}(r)\xrightarrow[r\to0]{}B_{lm}r^l\{1+[(2l-1)!!]^2\times(2l+1)\tan\eta_l/(kr)^{2l+1}\}, \tag{8}$$

where

$$B_{lm}=A_{lm}k^l/(2l+1)!!,$$

and in fact,

$$B_{lm}=\left(\frac{d}{dr}\right)^{2l+1}(r^{l+1}\psi_{lm})\bigg|_{r=0}. \tag{9}$$

Now, from the definition (7) of ψ_{lm}, we have

$$\begin{aligned}(\nabla^2+k^2)(Y_{lm}\psi_{lm})&=Y_{lm}\left[\nabla^2+k^2-\frac{l(l+1)}{r^2}\right]\psi_{lm}\\&=-Y_{lm}A_{lm}(\tan\eta_l)\left[\nabla^2+k^2-\frac{l(l+1)}{r^2}\right]n_l(kr)\\&=B_{lm}\left\{-\frac{[(2l+1)!!]^2}{k^{2l+1}}\tan\eta_l\right\}\frac{\delta(r)}{r^{l+2}}Y_{lm},\end{aligned} \tag{10}$$

which can be easily verified by integrating both sides of (10) over a small volume about the origin $r=0$. From (4) and (7),

$$\psi(\mathbf{r})=\sum_{l,m}Y_{lm}(\Omega)\psi_{lm}(r), \tag{11}$$

so that by combining (9), (10), and (11) one obtains the equation

$$\begin{aligned}(\nabla^2+k^2)\psi(\mathbf{r})=&\frac{4\pi}{-k\cot\eta_0}\delta(\mathbf{r})\frac{\partial}{\partial r}(r\psi)\\&+\sum_{l=1}^{\infty}\sum_{m=-l}^{+l}\left\{-\frac{[(2l+1)!!]^2}{k^{2l+1}}\tan\eta_l\right\}\\&\times\frac{\delta(r)}{r^{l+2}}\left(\frac{\partial}{\partial r}\right)^{2l+1}(r^{l+1}\psi_{lm})\lambda_{lm}(\Omega).\end{aligned} \tag{12}$$

The solution to the above equation then coincides with the actual wave function for $r\geqslant a$. We have thus succeeded in formulating the two-body hard sphere entirely in terms of measurable phase shifts.

It should be remembered that Eq. (11) may actually be incorrect inside the sphere $r=a$, as the right-hand side may fail to converge. However, if we neglect all phase shifts η_l with $l>L$, say, Eq. (12) would have only a finite number of terms on the right-hand side. The solution of such an equation would satisfy the boundary conditions at $r=a$ for all partial waves up to $l=L$. Equation (12) is therefore to be understood in the following sense: it is to be solved by first taking a finite number L of spherical harmonics and then approaching the limit $L\rightarrow\infty$.

The first term on the right-hand side of (12) represents the exact pseudopotential for S waves. If we expand its strength in powers of k^2:

$$\frac{1}{-k\cot\eta_0}=a+\tfrac{1}{2}(ka)^2(\tfrac{2}{3}a)+\cdots, \tag{13}$$

we see that the first term, the scattering length, was the only one included in the approximate equation (3). The next term involves the effective range $\frac{2}{3}a$, and is of the order a^3. If we contemplate a perturbation calculation in which a can be considered an expansion parameter, the first term above describes correctly effects up to the order a^2.

The other terms on the right-hand side of (12) give the contributions from higher partial waves. The strength of the lth multipole is

$$-\frac{[(2l+1)!!]^2}{k^{2l+1}}\tan\eta_l$$
$$=(2l+1)a^{2l+1}+\text{power series in } k^2. \tag{14}$$

Thus P-wave effects are of the order a^3, D-wave of the order a^5, etc. The lowest order term in each multipole is independent of k^2. If higher order terms are considered in a calculation, we may look upon k^2 as an operator whose effect on the wave function is given by the implicit equation

$$k^2\psi=\{-\nabla^2+\text{pseudopotentials}\}\psi, \tag{15}$$

so that through an iterative procedure we may understand, symbolically:

$$k^2=-\nabla^2+4\pi a\delta(\mathbf{r})\frac{\partial}{\partial r}r-\frac{4\pi}{3}a^3\delta(\mathbf{r})\nabla^2\frac{\partial}{\partial r}r+\cdots. \tag{16}$$

Equations (12), (15), and (16) define the pseudopotential for the two-body system under consideration. It yields the exact energy and the exact wave function for $r\geq a$.

It should be pointed out that the pseudopotential derived here is not a Hermitian operator. This should not cause any misgivings since the extended wave function is not supposed to represent a wave function for any physical system. It coincides, however, with the actual wave function except for a limited region of space which is of no physical interest. The non-Hermiticity of the pseudopotential requires that some care be exercised when one applies the usual perturbation formulas in an actual calculation.

(b) Illustrative Example

To illustrate the method of pseudopotentials introduced previously, we now apply it to a simple problem in which the exact solution is trivially known. By comparing the exact solution with an approximate solution obtained by treating the pseudopotentials as perturbations, we can hope to gain some familiarity with the method.

The example we shall discuss is the spherically symmetric solution of the wave equation

$$(\nabla^2+k^2)\psi=0, \tag{17}$$

with the boundary conditions

$$\psi=0 \quad\text{for}\quad r=R \quad\text{and}\quad r=a, \quad (R>a). \tag{18}$$

The normalized spherically symmetric solutions can be written down immediately:

$$\psi_n=[2\pi(R-a)]^{-\frac{1}{2}}\frac{\sin k_n(r-a)}{r}, \tag{19}$$

with eigenvalues

$$k_n=\pi n/(R-a),\quad n=1,2,3,\cdots. \tag{20}$$

This admits a power series expansion in a. In fact, by direct expansion of (19) and (20), we can write the wave functions as follows:

$$\psi_n=\psi_n^{(0)}+\psi_n^{(1)}+\psi_n^{(2)}+\cdots, \tag{21}$$

$$\psi_n^{(0)}=\frac{1}{\sqrt{(2\pi R)}}\frac{\sin\kappa_n r}{r},$$

$$\psi_n^{(1)}=-\frac{1}{\sqrt{(2\pi R)}}\frac{\kappa_n a}{r}\left[\left(1-\frac{r}{R}\right)\cos\kappa_n r-\frac{1}{2}\frac{\sin\kappa_n r}{\kappa_n R}\right], \tag{21a}$$

where $\kappa_n=\pi n/R$, and for the eigenvalues:

$$\begin{gathered}\epsilon_n=k_n^2=\pi^2n^2/(R-a)=\epsilon_n^{(0)}+\epsilon_n^{(1)}+\epsilon_n^{(2)}+\cdots,\\ \epsilon_n^{(l)}=(l+1)(a/R)^l\kappa_n^2.\end{gathered} \tag{21b}$$

For spherically symmetric solutions the S-wave pseudopotential exactly replaces the boundary condition at $r=a$, so that from (12), (13), and (16) the equation

$$(\nabla^2+k^2)\psi=\frac{4\pi}{-k\cot ka}\delta(\mathbf{r})\frac{\partial}{\partial r}(r\psi)$$
$$=4\pi a\delta(\mathbf{r})[1+\tfrac{1}{3}a^2\nabla^2+\cdots]\frac{\partial}{\partial r}(r\psi) \tag{22}$$

is exactly equivalent to (17) and (18). We can be certain that a perturbation calculation based on (22) with a as the expansion parameter gives, order by order, the correct solution to the problem, since we know that the actual problem admits a power series expansion in a. We want to demonstrate that such a perturbation calculation is also practicable by actually carrying it out.

To order a^2, we need only solve the equation

$$(\nabla^2+k^2)\psi=4\pi a\delta(\mathbf{r})\frac{\partial}{\partial r}(r\psi), \qquad \psi(R)=0. \tag{23}$$

We treat this equation by standard perturbation methods, using $\psi_n^{(0)}$ as our unperturbed wave functions, and treating as perturbing potential $U=4\pi a\delta(\mathbf{r})(\partial/\partial r)r$, whose matrix elements are

$$U_{mn}=\int\psi_m^{(0)}U\psi_n^{(0)}d\mathbf{r}=(2a\pi^2/R^3)mn. \tag{24}$$

Note that the factor $(\partial/\partial r)r$ in U is equal to unity when it acts on an unperturbed wave function.

The first-order energy correction is obtained at once:

$$\epsilon_n^{(1)}=U_{nn}=2a\pi^2n^2/R^3=(2a/R)\kappa_n^2, \tag{25}$$

which agrees with (21b). The first-order wave function is

$$\psi_n^{(1)}=\sum_{m\neq n}\frac{U_{mn}}{\kappa_n^2-\kappa_m^2}\psi_m^{(0)} =-\frac{1}{r}\frac{2an}{R\sqrt{(2\pi R)}}\sum_{m\neq n}\frac{m\sin m\theta}{m^2-n^2}, \tag{26}$$

where $\theta\equiv\pi r/R$. Upon summing the series in (26), one verifies the agreement between (26) and (21).

The second-order energy is then obtained by

$$\epsilon_n^{(2)}=\int\psi_n^{(0)}U\psi_n^{(1)}d\mathbf{r}. \tag{27}$$

It is important that we evaluate the above integral by putting in the closed form of $\psi_n^{(1)}$ from (21a), instead of letting U operate on its series representation (26) term by term (leading to a divergent integral). The factor $(\partial/\partial r)r$ in U is now essential. It just serves to "weed out" the singular $1/r$ term in $\psi_n^{(1)}$, giving finally a finite second-order energy

$$\epsilon_n^{(2)}=3(a/R)^2\kappa_n^2,$$

in agreement with (21).

The third-order perturbation calculation can also be carried out. One must include now the contribution (of order a^3) of the effective range to the pseudopotential. It is easily shown that when this is done, one again obtains the correct third-order energy.

3. MANY-BODY PROBLEM

(a) Formulation of the Pseudopotential in the Many-Body System

We consider a system of N particles, each of mass m, enclosed in a cubical volume V, with two-body hard-sphere interactions. The Schrödinger equation for the system is

$$\begin{aligned}&[(\hbar^2/2m)(\nabla_1^2+\nabla_2^2+\cdots+\nabla_N^2)+E]\Psi(1\cdots N)=0 \\ &\qquad\qquad\text{for } r_{ij}>a, \quad \text{all } i\neq j, \\ &\Psi(1\cdots N)=0 \quad \text{for } r_{ij}\leqslant a, \quad \text{any } i\neq j,\end{aligned} \tag{28}$$

where $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$. We have used the abbreviation $1\cdots N$ to denote the set of coordinates $\mathbf{r}_1\cdots\mathbf{r}_N$, plus spin or isotopic spin coordinates, if any. The boundary condition at large distances will be taken to be the usual periodic boundary conditions in a cubical box of volume $V=L^3$.

Before going into any formal considerations, it would be helpful to interpret the hard-sphere boundary conditions in a geometrical way. Consider the $3N$-dimensional configuration space of the system. The subspace defined by the condition $r_{ij}=a$, for example, is a "cylindrical" surface which is easy to visualize. There are altogether $\frac{1}{2}N(N-1)$ such cylinders in the configuration space. Taken together, they represent a complicated but well-defined tree-like surface, on which the wave function must vanish.

To help visualization, we may try to draw a part of this "tree," in a very schematic way, as in Fig. 2. The cylinder labeled 12, for example, represents the region for which $r_{12}=a$, while coordinates other than $\mathbf{r}_1$, $\mathbf{r}_2$ are free to vary. Similarly, the surface formed by the intersection between the cylinders 12 and 13 represents the configuration for which $r_{12}=a$, $r_{13}=a$, while all coordinates other than $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$ are free to vary.

A way of reformulating the problem immediately suggests itself. It would probably be instructive at this

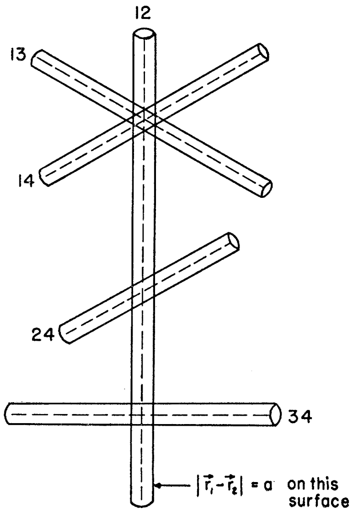

FIG. 2. Schematic representation of the "tree"-like surface in $3N$-dimensional configuration space on which $\Psi=0$, as required by the hard-sphere interactions among the particles.

point to recall the previous treatment of the two-particle problem and visualize it in a similar geometrical fashion. There the "tree" was in fact the sphere $r=a$. The introduction of the pseudopotential amounts to nothing more than considering the surface "charge" induced on this sphere, and then making a multipole expansion of the surface charge. As long as we stay outside of the sphere, the wave function is correctly given by that produced by a series of multipoles placed at the origin, with multipole strength appropriately chosen.

In the many-body case, the same physical idea may be applied. We can regard the boundary condition that

$$\Psi=0 \text{ on the surface of the "tree,"}$$

as equivalent to the existence of induced "charges" on the surface of the "tree." It would then be natural to make a multipole expansion of this surface charge, namely, to replace it by multipoles along the "axial lines" of the "tree."

Mathematically, we can formulate the above idea as follows: Define first a Green's function $G(\mathbf{r}_1\cdots\mathbf{r}_N,\mathbf{r}_1'\cdots\mathbf{r}_N')$ by

$$[(\hbar^2/2m)(\nabla_1^2+\cdots+\nabla_N^2)+E]G(\mathbf{r}_1\cdots\mathbf{r}_N,\mathbf{r}_1'\cdots\mathbf{r}_N') \\ =-4\pi\delta(\mathbf{r}_1-\mathbf{r}_1')\cdots\delta(\mathbf{r}_N-\mathbf{r}_N'). \quad (29)$$

Then, by Green's theorem,

$$\Psi(1\cdots N)=\Phi(1\cdots N)+\int G(\mathbf{r}_1\cdots\mathbf{r}_N,\mathbf{r}_1'\cdots\mathbf{r}_N') \\ \times\left[\frac{1}{4\pi}\frac{\partial}{\partial n}\Psi(1'\cdots N')\right]dT', \quad (30)$$

where Φ satisfies everywhere the equation

$$[(\hbar^2/2m)(\nabla_1^2+\cdots+\nabla_N^2)+E]\Phi=0, \quad (31)$$

and $\partial/\partial n$ denotes the normal derivative with respect to the "tree." The integral in (30) is extended over the surface of the "tree" for which dT' is a surface element. The boundary condition at infinity for G and Φ can be arbitrary as long as they lead to the correct asymptotic behavior of Ψ as given with (28).

The expression $[(1/4\pi)\partial\Psi/\partial n]$ can thus be interpreted as the surface charge density induced on the "tree" as a consequence of the boundary condition. We can decompose the surface integral in (30) into a sum of integrals over the various branches of the "tree." The simplest branches are, of course, the "cylinders" $r_{ij}=a$, corresponding to effects of binary collisions. The multipole expansion for these branches reduces to the two-body problem we had previously discussed, and the pseudopotentials due to the "axial multipoles" for these branches can be written down immediately. Thus, with only binary collisions taken into account, the extended wave function satisfies the equation

$$(H_0+H')\Psi=E\Psi, \quad (32)$$

where

$$H_0=-(\hbar^2/2m)(\nabla_1^2+\cdots+\nabla_N^2),$$

and H' is $(-\hbar^2/m)$ times the operator on the right-hand side of (12), summed over all pairs of relative distances r_{ij}, with k^2 interpreted by an obvious generalization of (15) and (16). We shall display H' only to the lowest order in a:

$$H'=\frac{4\pi a\hbar^2}{m}\sum_{i<j}\delta(\mathbf{r}_i-\mathbf{r}_j)\frac{\partial}{\partial r_{ij}}r_{ij}. \quad (33)$$

One notes that the pseudopotential H' is not Hermitian. It is, of course, understood that while we have now extended the wave function Ψ into the region in the interior of the "tree," only the solution of Ψ outside the "tree" coincides with the actual wave function and has physical meaning. The attitude we take here regarding the convergence of the multipole expansion is the same as that for the two-body case previously discussed, namely, that we must first ignore all multipoles higher than a given order L, solve the equations, and then let L approach infinity.

The effects of collisions higher than binary can only be estimated in a rough way. For example, the effect of the three hard spheres 1, 2, and 3 simultaneously colliding will be represented in our geometrical picture by the multipole required at the intersection of cylinders 12 and 13. By a dimensional argument, one expects the lowest pole order (monopole) required there to be of at least order a^4. Similarly, the effects of four hard spheres simultaneously colliding will be at least of order a^7. Consequently, in a perturbation calculation in which orders are classified by the powers of a, the expression H' given in (33) correctly accounts for effects up to and including a^2.

Instead of going further into the question of the exact pseudopotential to be used for the many-body system, together with such questions as convergence and rigor, we shall now assume that at least under certain circumstances it is meaningful to speak of a power series expansion of physically interesting quantities in powers of a. We shall then treat the pseudopotential as a perturbation, and examine the consequences of a perturbation calculation which includes effects up to order a^2 only. Accordingly, H' as given by (33) will be the perturbation Hamiltonian adopted for the remaining part of the investigation.

(b) First Order Energy for a Bose System

We consider as the unperturbed system a free Bose gas consisting of N particles, of mass m each, in volume V. The unperturbed wave functions and energy levels are therefore, respectively,

$$\begin{aligned}\Psi_n^{(0)}&=\mathcal{S}e^{i(\mathbf{k}_1\cdot\mathbf{r}_1+\cdots+\mathbf{k}_N\cdot\mathbf{r}_N)}V^{-N/2},\\ E_n^{(0)}&=\textstyle\sum_\alpha n_\alpha(\hbar^2k_\alpha^2/2m),\end{aligned} \quad (34)$$

where $\mathbf{k}_1 \cdots \mathbf{k}_N$ are the momenta of the particles, n_α are the occupation numbers for the momentum states, and $\mathcal{S}$ is the symmetrizing operator. The index n stands for the set of occupation numbers. The periodic boundary conditions in a cubical box requires that each momentum vector be of the form

$$\mathbf{k} = (2\pi/L)(m,n,l), \quad L = V^{\frac{1}{3}}, \tag{35}$$

where m, n, l, are $\pm$ integers. The pseudopotential (33) is treated as a perturbation on this system.

For the sake of calculations, it is often convenient to go over to the equivalent description of a many-body system in the language of quantized fields. As usual, one introduces the field operator $\psi(\mathbf{r})$ which can be expanded in a Fourier series:

$$\psi(\mathbf{r}) = V^{-\frac{1}{2}} \textstyle\sum_\alpha a_\alpha e^{i\mathbf{k}_\alpha \cdot \mathbf{r}}, \tag{36}$$

where a_α, $a_\alpha{}^*$, respectively, denote the annihilation and creation operator for the single particle state of momentum $\mathbf{k}_\alpha$, with commutation rules

$$[a_\alpha, a_\beta{}^*] = \delta_{\alpha\beta}, \tag{37}$$

as is appropriate for Bose statistics. The perturbation Hamiltonian can then be written

$$H' = \left(\frac{4\pi a\hbar^2}{m}\right)\frac{1}{2}\int d\mathbf{r}_1 d\mathbf{r}_2 \psi^*(\mathbf{r}_1)\psi^*(\mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_2) \times \frac{\partial}{\partial r_{12}}[r_{12}\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)]. \tag{38}$$

Noting that the differential operator $(\partial/\partial r)r$ is equal to unity when it acts on the unperturbed state, one gets, for the first order energy:

$$\begin{aligned} E_n{}^{(1)} &= (\Psi_n{}^{(0)}, H'\Psi_n{}^{(0)}) \\ &= (4\pi a\hbar^2/m)\tfrac{1}{2} \sum_{\alpha\beta\gamma\lambda} (\Psi_n{}^{(0)}, a_\alpha{}^* a_\beta{}^* a_\gamma a_\lambda \Psi_n{}^{(0)}) \\ &\qquad \times \langle \alpha\beta | \delta(\mathbf{r}_1 - \mathbf{r}_2) | \gamma\lambda \rangle, \end{aligned} \tag{39}$$

where

$$\langle \alpha\beta | \delta(\mathbf{r}_1 - \mathbf{r}_2) | \gamma\lambda \rangle = V^{-1}\delta(\mathbf{k}_\alpha + \mathbf{k}_\beta - \mathbf{k}_\gamma - \mathbf{k}_\lambda), \tag{40}$$

where the δ function of the momenta above is a Kronecker delta, expressing the conservation of total momentum. One easily obtains[6]

$$E_n{}^{(1)} = (4\pi a\hbar^2/mV)(N^2 - \tfrac{1}{2}N - \tfrac{1}{2}\textstyle\sum_\alpha n_\alpha{}^2). \tag{41}$$

For the ground state of the total system, this correction is[7]

$$E_g{}^{(1)} = (2\pi a\hbar^2/m)(N/V)N. \tag{42}$$

The form of the first order energy, expression (41), can be understood in physical terms. The first term, proportional to $aN(N/V)$, is that expected on the basis of an "index of refraction approximation." If we imagine each particle to move through the system as if the latter were a uniform optical medium, we can expect each particle to have an increment in energy proportional to $n^2 - 1$, where n is the index of refraction. Now for a medium of low density, a classical result of Lagrange states that

$$n^2 - 1 \propto N/V.$$

From this picture, therefore, one expects the energy increment of the total system to be proportional to $N(N/V)$. In a more detailed interpretation of the present case, we may say that at very low energies, the interaction between particles is shape-independent, and is characterized by only a single parameter, the scattering length a. We may therefore replace the actual interparticle potential by a square well of such radius and depth that it gives rise to the same scattering length. To a single particle which moves through the system, the square wells presented by the remaining $N-1$ particles may overlap to form a constant potential, whence the medium-like behavior of the system. The depth of this effective constant potential is of course proportional to the scattering length a.

The last term in (41), of the form $-\sum_\alpha n_\alpha{}^2$, is purely quantum mechanical in origin. By virtue of this term, the energy increment of the system due to the hard-sphere repulsions is smallest when all particles are in the same momentum state. In other words, the particles tend to condense into the same momentum state in order to minimize the spatial repulsion; i.e., *spatial repulsion leads to momentum-space condensation.*[8] This is a consequence of the Heisenberg uncertainty principle applied to the canonically conjugate pair: relative momentum and relative distance of two particles.

One further notes an interesting property of the first order energy. For the low-lying states of the system, the only important term in the sum $\sum_\alpha n_\alpha{}^2$ is the single-particle ground state contribution, namely $n_0{}^2$. One can write the first order energy levels of the system, to a good approximation, as

$$E_n = \textstyle\sum_\alpha n_\alpha(\hbar^2 k_\alpha{}^2/2m) + (4\pi a\hbar^2/mV)(N^2 - \tfrac{1}{2}n_0{}^2). \tag{43}$$

To change the number n_0 of particles in the ground state by one unit would require a finite amount of energy

$$\Delta = (4\pi a\hbar^2/m)(n_0/V). \tag{44}$$

The energy level spectrum of the entire system therefore consists of a series of continua, each separated from the others by finite energy gaps, as indicated in Fig. 3. If a very small amount of energy is applied externally to excite the system, all one can do is to induce transitions

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[6] Equation (41) was obtained by a different method in 1953 by Luttinger and Yang (unpublished). Dr. P. Price subsequently informed us that he had obtained the same expression independently [P. Price, thesis, Cambridge University, Cambridge, 1951 (unpublished)].

[7] W. Lenz, Z. Physik **56**, 778 (1929) has given a formula equivalent to (42) for the ground state of a particle moving through the field of the other particles which are held fixed.

[8] This is a well-known point. See, for example, F. London, *Superfluids* (John Wiley and Sons, Inc., New York, 1954), Vol. 2, p. 39.

in which only particles not in the ground state are affected. In this sense, the system exhibits some properties of a superfluid, in that a part of the system, i.e., the particles in the ground state, will not exhibit such properties as viscosity until energies higher than a critical amount Δ is transferred to the system. Note that the energy gap is a function of n_0. Note further that the first order energy here, on account of the quantum mechanical term, cannot in any sense be imagined to be a simple sum over N single-particle contributions. It involves the cooperative contribution of all the particles.[9]

The above discussion, based on the first order energy alone, is to be taken as suggestive rather than conclusive. It serves to point out that as a result of the hard-sphere interactions, the energy level density of a Bose gas near the ground state may experience violent changes.

(c) Second and Third Order Energies

The ground state energy of a Bose gas with hard-sphere interactions can be calculated to third order with the pseudopotential H' given by (33). The contribution to the pseudopotential from the effective range parameter, normally or order a^3 [see (13)], vanishes for the ground state, where all particles have zero momentum in the unperturbed system. For the Bose gas considered here, P-wave scattering is evidently absent.

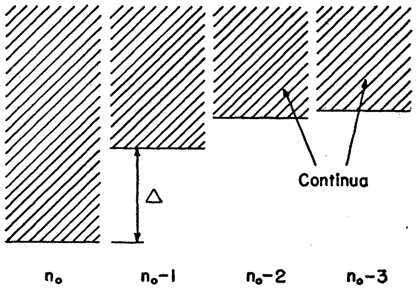

FIG. 3. Energy levels of the system of Bose particles with hard-sphere interactions according to the first-order formula (43). The levels may be grouped into continua, each labeled by n_0, the number of particles in the single-particle ground state. Successive continua are separated by an energy gap Δ, given by (44).

We shall need the first-order correction $\Psi_g^{(1)}$ to the ground state wave function of the system:

$$\Psi_g^{(1)}=\sum_{n\neq g}\frac{(\Psi_n^{(0)},H'\Psi_g^{(0)})}{-E_n^{(0)}}\Psi_n^{(0)}, \tag{45}$$

where the unperturbed ground state wave function is just a constant:

$$\Psi_g^{(0)}=V^{-N/2},\quad E_g^{(0)}=0. \tag{46}$$

The only nonvanishing matrix elements of H' appearing in (45) connects the ground state to states $\Psi_n^{(0)}$ in which two particles, say α and β, are excited with equal and opposite momenta:

$$\mathbf{k}_\alpha=-\mathbf{k}_\beta=\mathbf{k},$$

while all other $N-2$ particles remain in the single-particle ground state. We may use the vector $\mathbf{k}$ to label the excited wave functions, and find

$$(\Psi_{\mathbf{k}}^{(0)},H'\Psi_g^{(0)})=(4\pi a\hbar^2/mV)[N(N-1)]^{\frac{1}{2}}, \tag{47}$$

where

$$\Psi_{\mathbf{k}}^{(0)}=[N(N-1)]^{-\frac{1}{2}}V^{-N/2}\sum_{i\neq j}e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}. \tag{48}$$

Therefore,

$$\Psi_g^{(1)}=-(4\pi a/V)\sum_{i<j}F(\mathbf{r}_{ij})\Psi_g^{(0)}, \tag{49}$$

where

$$F(\mathbf{r})\equiv\sum_{\mathbf{k}\neq 0}e^{i\mathbf{k}\cdot\mathbf{r}}/k^2. \tag{50}$$

The $\mathbf{k}$ sum above extends over all momentum vectors of the form (35), except zero.

It is easy to show that $F(\mathbf{r})$ satisfies the equation

$$\nabla^2F(\mathbf{r})=-4\pi\rho(\mathbf{r}), \tag{51}$$

where

$$\rho(\mathbf{r})=(V/4\pi)[\delta(\mathbf{r})+\sum_{\mathbf{n}\neq 0}\delta(\mathbf{r}+\mathbf{n}L)-1/V], \tag{52}$$

with $\mathbf{n}$ a vector whose components are ± integers. Hence $F(\mathbf{r})$ is $(V/4\pi)$ times the electrostatic potential at the point $\mathbf{r}$, due to a cubic lattice of unit positive point charges immersed in a uniform negative charge of density $1/V$ (see Fig. 4). The lattice constant being L, the total charge in a unit cell is zero.

The behavior of $F(\mathbf{r})$ near $\mathbf{r}=0$ can be readily obtained. Since the charge distribution in each cell has cubic symmetry, the electrostatic potential due to each cell drops off outside of the cell at least as fast as that due an electric 2^4 pole. Therefore, near $\mathbf{r}=0$, i.e., near the center of a particular cell, the contribution to $F(\mathbf{r})$ comes almost entirely from the point positive charge of that cell and the cubical block of its own negative

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[9] It must be pointed out, however, that the formula (41) is not exact, even to first order. This is because the unperturbed energy levels are degenerate. Instead of describing the splitting of the levels under the perturbation, (41) gives only the "center of gravity" of the split levels. This fact in itself is of no great consequence, since in dealing with a system of a large number of particles, for example in the evaluation of the partition function, it is only the behavior of the system averaged over levels that is important. However, the fact that the degeneracy is not removed in first order means that one must exercise caution in going to higher order approximations. Second and higher order approximations, therefore, can only be carried out for the lowest state, which is not degenerate.

It should further be pointed out that formula (41), when taken literally, would lead to the crossings of the levels as the diameter a becomes of the order of $V^{\frac{1}{3}}/N$, which in turn means that the perturbation calculation breaks down for larger values of a. This shows the intrinsic limitation in the applicability of the formula to the case of finite densities. However, it may be emphasized that (41) does not lead to a crossing of the ground state with any other state. Perturbation calculations, therefore, can be expected to be better for the ground state.

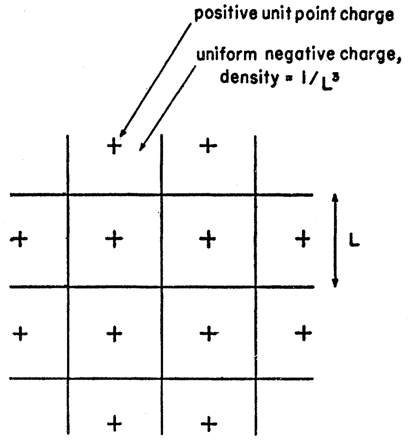

FIG. 4. The charge distribution whose electrostatic potentia is equal to the function $F(\mathbf{r})$ appearing in the first-order wave function (49).

charge, which can be easily calculated. One finds

$$F(\mathbf{r})\underset{r\to 0}{\longrightarrow}\frac{V}{4\pi}\left(\frac{1}{r}-\frac{C}{L}\right), \tag{53}$$

where C is a constant reminiscent of Madelung's constant in the theory of ionic crystals, and is found to be

$$C=2.37. \tag{54}$$

The second order energy for the ground state is then given by

$$\begin{aligned}E_g^{(2)}=(\Psi_g^{(0)},H'\Psi_g^{(1)})&=-\left(\frac{4\pi a\hbar^2}{m}\right)\left(\frac{4\pi a}{V}\right)\\&\quad\times\frac{N(N-1)}{2}\int\frac{d\mathbf{r}}{V}\delta(\mathbf{r})\frac{\partial}{\partial r}[rF(\mathbf{r})]\\&=2.37(a/L)E_g^{(1)}.\end{aligned} \tag{55}$$

Therefore, for any reasonably large volume, $E_g^{(2)}$ is essentially zero.

The third order energy correction for the ground state may be calculated by means of the general perturbation formula

$$E_n^{\prime 3)}=-(\Psi_n^{(1)},\Psi_n^{(1)})E_n^{(1)}+\left(\Psi_n^{(0)},H'\sum_{m\neq n}\frac{(\Psi_m^{(0)},H'\Psi_n^{(1)})}{E_n^{(0)}-E_m^{(0)}}\Psi_m^{(0)}\right). \tag{56}$$

The calculation is straightforward, and we shall merely quote the result:

$$E_g^{(3)}=[(2.37)^2+(\xi/\pi^2)(2N-5)](a/L)^2E_g^{(1)}, \tag{57}$$

where

$$\xi\equiv\sum_{l,m,n=-\infty}^{+\infty}{}'\frac{1}{(l^2+m^2+n^2)^2}.$$

The prime in the summation above means the omission of the term with $l=m=n=0$. The third order energy $E_g^{(3)}$ is small compared to the first order energy only if $N(a/L)^2\ll 1$. The question of the meaning of this perturbation expansion of the energy levels will be discussed in Sec. 4.

(d) Fermi Statistics

One can also treat a system of fermions with hard-sphere interactions by the method of pseudopotentials. The pseudopotential H', correct to order a^2, is also given by (33). In the quantized field language, H' can also be written in the form (38), with the field operator $\psi(\mathbf{r})$ defined by (36), except that the commutators (37) should be replaced by anticommutators. The result of a perturbation calculation will now be summarized.

We consider a system of N fermions with spin and isotopic spin variables. It is possible for the wave function to be symmetric under the spatial exchange of some pairs of particles, so that binary S-wave collisions exist. The unperturbed wave function is as usual a Slater determinant of the following single-particle wave functions with periodic boundary conditions:

$$u_\alpha(\mathbf{r},\sigma,\tau)=V^{-\frac{1}{2}}e^{i\mathbf{k}_\alpha\cdot\mathbf{r}}\delta(s_\alpha,\sigma)\delta(t_\alpha,\tau), \tag{58}$$

where σ, τ are, respectively, the spin and isotopic coordinates, which may assume values $+1, -1$. The quantum number labeling the spin state is s_α and that for the isotopic spin state, t_α. They also assume values $+1$ or -1. The spin and isotopic spin eigenfunctions are the Kronecker deltas $\delta(s_\alpha,\sigma)$, $\delta(t_\alpha,\tau)$ in (58). The two single-particle eigenstates of isotopic spin will be called "proton" and "neutron" states. The unperturbed energy is still given by (34); but the occupation numbers n_α are now either 0 or 1. For the ground state of the system with equal numbers of "protons" and "neutrons" in a large volume:

$$E_g^{(0)}=\frac{9\pi}{40}\left(\frac{16\pi}{3}\right)^{\frac{1}{3}}\frac{\hbar^2}{m}\left(\frac{N}{V}\right)^{\frac{2}{3}}N, \tag{59}$$

as is well known.

The first-order energy is given by

$$\begin{aligned}E_n^{(1)}=(\Psi_n^{(0)},H'\Psi_n^{(0)})&=\tfrac{1}{2}(4\pi a\hbar^2/m)\\&\quad\times\textstyle\sum_{\alpha\beta}n_\alpha n_\beta[\langle\alpha\beta|\delta(\mathbf{r}_1-\mathbf{r}_2)|\alpha\beta\rangle\\&\qquad-\langle\alpha\beta|\delta(\mathbf{r}_1-\mathbf{r}_2)|\beta\alpha\rangle]\\&=(2\pi a\hbar^2/mV)[N^2-\textstyle\sum_{\alpha\beta}n_\alpha n_\beta\delta(s_\alpha,s_\beta)\delta(t_\alpha,t_\beta)],\end{aligned} \tag{60}$$

which gives for the ground state of the system

$$E_g^{(1)}=\frac{3}{2}\frac{\pi a\hbar^2}{m}\left(\frac{N}{V}\right)N, \tag{61}$$

which is of the same form as that for the Bose case except for a numerical factor of $\frac{3}{4}$. The origin of this factor is clear. It represents the fraction of the particles that can interact in the S state with a given particle.

The calculation of the second order energy for the ground state is considerably more involved than the Bose case, because the Fermi ground state has a more complicated structure than that for the Bose system. We shall not go into the details here, but shall merely indicate a few steps in the calculation. In a manner analogous to (55), we now have

$$E_g^{(2)}=\frac{6\hbar^2}{m}\left(\frac{4\pi a}{V}\right)^2\sum_{\mathbf{k}_\gamma,\mathbf{k}_\lambda}^{\text{occ.}}\frac{\partial}{\partial r}[rf(\mathbf{k}_\gamma\mathbf{k}_\lambda\,|\,\mathbf{r})]_{r=0}, \tag{62}$$

where

$$f(\mathbf{k}_\gamma\mathbf{k}_\lambda\,|\,\mathbf{r})=\sum_{\mathbf{k}_\alpha,\mathbf{k}_\beta}^{\text{occ.}}\frac{e^{i\mathbf{k}_{\alpha\beta}\cdot\mathbf{r}}}{k_{\gamma\lambda}^2-k_{\alpha\beta}^2},\quad \mathbf{k}_{\alpha\beta}\equiv\tfrac{1}{2}(\mathbf{k}_\alpha-\mathbf{k}_\beta), \tag{63}$$

with the restrictions

$$\mathbf{k}_\alpha\neq\mathbf{k}_\beta\neq\mathbf{k}_\gamma\neq\mathbf{k}_\lambda,$$
$$\mathbf{k}_\alpha+\mathbf{k}_\beta=\mathbf{k}_\gamma+\mathbf{k}_\lambda.$$

The sums in (62), (63) are to be extended over occupied momenta in the ground state of the system. The explicit calculation of the second energy is extremely tedious. For a very large volume of the system, the result is

$$E_g^{(2)}=1.30a(N/V)^{\frac{1}{3}}E_g^{(1)}. \tag{64}$$

Comparing this to the corresponding formula (55) for the Bose case, we see that there is an extra factor $N^{\frac{1}{3}}$, which comes from the extra parameter absent in the Bose case, namely, the momentum of the Fermi level.

4. DISCUSSION

We shall attempt to give in this section a critical discussion of the range of applicability of the method developed above.

(A) For the two-body problem with arbitrary given boundary condition at large relative distance, i.e. the problem discussed in Sec. 2(a), the method enables one to calculate, in principle, the exact energy levels and the exact wave functions outside the range of interaction. The information needed for the calculation are the phase shifts η_l as functions of the relative momentum k. It is clear that the method is applicable in this case for any interaction $V(r)$ between the two bodies, provided that if $V(r)$ is continuously distorted so that $\eta_l\rightarrow 0$, the wave functions approach the free-particle wave functions. This last condition is evidently true for the hard-sphere interaction. It is in fact true for any $V(r)$ that does not give rise to a bound state. This exclusion of interactions that give rise to bound states is physically important. A given set of phase shifts correspond to a whole series of potentials, each differing from the others by the number of bound states it allows.[10] The method developed in this paper depends only on the phase shifts, and is applicable only to the potential with no bound states.

(B) For the many-body problem the method contains an intrinsic difficulty concerning the effect of three-body collisions discussed in Sec. 3(a). It can therefore only give approximate results insofar as such effects can be neglected. It is believed, however, that such effects are of order a^4 or higher.

In addition, the following condition, similar to the one discussed above, must be satisfied by the interaction $V(r)$: that if $V(r)$ is continuously distorted so that the two-body phase shifts $\eta_l\rightarrow 0$, the many-body wave functions must approach the free-particle wave functions. In other words, there must be no many-body bound states.

An important question that arises in the many-body problem is: what is the dimensionless parameter of expansion in the perturbation calculation? One especially wants to know the N dependence of the different terms in the perturbation series, and whether the series is meaningful for finite values of a and (N/V) in the limit that $N\rightarrow\infty$. We do not know the answer to these questions.

However, the perturbation series is meaningful if we consider N to be fixed while V assumes sufficiently large values. It is therefore entirely possible that a better treatment would result if we divide the total system into smaller subsystems and apply these methods only to the subsystems, while the long-range correlation between subsystems would be treated by a method analogous to the method of classical hydrodynamics.

Another possibility which suggests itself is that since the perturbation series is certainly valid for fixed N and infinitely large V, these methods are particularly adapted to a calculation of virial coefficients. Such a calculation is indeed practicable, and will be the subject of a separate paper.[11]

ACKNOWLEDGMENT

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[10] R. Jost and W. Kohn, Phys. Rev. **87**, 977 (1952).

[11] Huang, Yang, and Luttinger, following paper [Phys. Rev. **105**, 776 (1957)].