liquid nitrogen, Compton scattering causes degradation in the energy of some of the 511-kev gamma rays. This is probably the reason that no three-quantum radiation was observed in an earlier experiment.[7]

From the change in the ratio of peak to valley counting rates, and the resolution curve of the spectrometer, the abundance of three-quantum events may be calculated. The abundance of three-quantum annihilation in liquid helium is $(16\pm3)\%$. This amount of three-quantum annihilation radiation clearly indicates that the τ_3 component is due to orthopositronium.

Triple-coincidence measurements were made to verify the existence of orthopositronium. Three NaI scintillation counters were placed coplanar with the source every 120° around the source. The triple-coincidence rate was compared with the rate in liquid nitrogen. The coincidence rate in helium was greater than that in nitrogen by (0.7 ± 0.2) count per minute. From this coincidence rate, the abundance of three-quantum annihilation is $(13\pm4)\%$. This is in satisfactory agreement with the abundance calculated from the gamma-ray spectrum analysis.

DISCUSSION

The three mean lives, τ_1, τ_2, and τ_3 are associated with parapositronium, free positron annihilation, and orthopositronium annihilation, respectively. The orthopositronium component has an abundance of $16\pm2\%$, based on the three abundances listed above. Any error in the mean life τ_3 would affect this value. If τ_3 is smaller than 1.2×10^{-7} sec, the abundance would be increased. If the long-lived component is due to orthopositronium, the very short-lived one must be due to parapositronium, and will have an abundance of about 5%. The remaining 79% of the positrons do not form positronium.

The mean life of the short-lived component, $\tau_1<5\times10^{-10}$ sec, indicates that positrons rapidly lose energy in liquid helium, so that in a time less than 5×10^{-10} sec the positron has either formed positronium or has lost so much energy that positronium formation is no longer possible. The intermediate mean life, $\tau_2=2.6\times10^{-9}$ sec, is longer than that generally found for free positrons in condensed materials. The component of long mean life, $\tau_3=1.2\times10^{-7}$ sec, indicates that very little pickoff annihilation occurs. From this it may be concluded that the exchange repulsion between the positronium atom and the helium atom is much stronger than any polarization effects which would tend to raise the electron density at the positron.

The behavior of positrons in liquid helium is just about what would be expected in helium gas at the same density, i.e., about 700 atmospheres at 0°C. Computation of the annihilation probability for free positrons using Ore's correction for Coulomb effects[4] for helium gas at 700 atmospheres gives a mean life which is in exact agreement with the value measured. The fraction of the positrons forming positronium is consistent with the predictions of Ore[4] and with the triple-coincidence studies of helium gas by de Benedetti and Siegel.[6]

[7] F. L. Hereford, Phys. Rev. 95, 1097 (1954).

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Ground-State Energy of a Hard-Sphere Gas

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Rigorous lower and upper bounds are established for the energy of the ground state of a Bose gas with hard-sphere interaction between particles.

1. STATEMENT OF RESULTS

We consider a Bose gas consisting of N identical nonrelativistic particles in a cubical box of volume V. Between each pair of particles there is a hard-sphere repulsion of range a, and no other interaction. Let m be the mass of each particle, and $\rho=N/V$, $\rho_1=(N-1)/V$. We suppose $N\geq 2$.

Let E be the ground-state energy of the gas. Calculations by Lee and Yang[1] have shown that

$$E\sim[2\pi\hbar^2N\rho a/m], \qquad (1)$$

as $N\to\infty$ and $a\to0$. The meaning of Eq. (1) is that as $a\to0$ the error is of higher than first order in a. An asymptotic formula of this kind has the disadvantage that there seems to be no way to convert it into a precise inequality. The error introduced by breaking off the asymptotic expansion in powers of a at any term is not controllable; it is unlikely that the power series converges in the strict sense for any value of a.

The purpose of this paper is to supplement Eq. (1) with precise inequalities.

Theorem 1.— $$E>[\tfrac{1}{10}\sqrt{2}\pi\hbar^2N\rho a/m]. \qquad (2)$$

[1] T. D. Lee and C. N. Yang (private communication).

This lower bound for E is absurdly weak compared with Eq. (1). The result is of interest only because it is proved in a completely elementary and rigorous way, and because it holds irrespective of the magnitude of N and a.

The ground-state wave function is a function

$$\Psi(r_1,\cdots,r_N) \tag{3}$$

of the positions of the N particles. If the walls of the box are impenetrable, Ψ vanishes when any r_i is at the boundary of the box. In this case we can extend the definition of Ψ to a continuous periodic function having the edge of the box for period in every coordinate. Thus Eq. (2) will hold for an impenetrable box if it holds for a box with periodic boundary conditions. We shall prove Theorem 1 for the more general case of periodic boundary conditions. In this way we avoid having to discuss the inessential complications arising from boundary effects.

We prove a second theorem establishing a lower bound for E which is potentially much stronger than Theorem 1. However, this second bound is expressed in terms of a two-particle distribution-function which we are not able to evaluate explicitly. Henceforth we always assume periodic boundary conditions. We define the function

$$R_i=R_i(r_1,\cdots,r_N) \tag{4}$$

to be the distance of the point r_i from its nearest neighbor among the r_j, measuring the distance "across the boundary" into the next period whenever necessary. Let $P(u)$ be the probability-distribution of the quantity R_i^3 in the ground-state of the gas. Explicitly,

$$P(u)=\int|\Psi|^2\delta[R_i^3-u]d\tau_1\cdots d\tau_N. \tag{5}$$

Clearly $P(u)$ is independent of i, and is a continuous function of u defined on the finite interval $a\leq u\leq V^{\frac{1}{3}}$, with $\int P(u)du=1$.

Theorem 2.— $E>[3\hbar^2Na/2m]\max_u P(u)$. (6)

The interest of Theorem 2 arises from the fact that, for a perfect Bose gas in an infinitely large box ($a=0$ and $N=\infty$), we have

$$P(u)=[(4/3)\pi\rho]\exp[-(4/3)\pi\rho u],\quad \max_u P(u)=(4/3)\pi\rho. \tag{7}$$

For a perfect gas with finite N,

$$\max_u P(u)=P(0)=(4/3)\pi\rho_1. \tag{8}$$

It is plausible to imagine that the presence of a hard-sphere repulsion will compress the probability distribution $P(u)$ into a shorter interval and so increase the value of $[\max_u P(u)]$ above the perfect gas value. Thus Eq. (6) leads to the conjecture that for all values of a and N

$$E>[2\pi\hbar^2N\rho_1 a/m], \tag{9}$$

and suggests a way in which this conjecture may subsequently be proved.

The third theorem deals with the much easier problem of the upper bound. The upper bound is easier because the true energy is the minimum expectation value of the Hamiltonian of the system. So the problem reduces to finding an approximate wave function which is (a) a good approximation to the true ground state, and (b) simple enough to make precise calculation possible. Requirements (a) and (b) obviously work against each other, and the choice of a wave function demands a compromise. We have chosen our wave function [Eq. (35) below] in the belief that it satisfies (a) better than (b). That is to say, we believe that the exact expectation value of the Hamiltonian for our wave function would be much closer to the true ground-state energy than to the best upper bound which we have been able to calculate for it.

Theorem 3.—

$$E<\left[\frac{2\pi\hbar^2N\rho_1 a}{m}\right]\left[\frac{1+2(a/b)}{(1-(a/b))^2}\right],\quad a<b, \tag{10}$$

with the length b independent of a and defined by

$$(4/3)\pi b^3\rho_1=1. \tag{11}$$

According to Eq. (11), b^3 is the mean cube of the distance of a particle from its nearest neighbor, when N particles are placed at random in the volume V.

Theorem 3 states nothing when $a>b$. Our wave function [Eq. (35)] is clearly inappropriate to describe the state of affairs as a approaches the "jamming radius" $a_J=1.81b$ at which the spheres become rigidly fixed in a closed-packed lattice. For $b\leq a<a_J$ it would be better to use a trial wave function of a "crystalline" form, in which each particle vibrates about a fixed center, and the centers form a regular crystal lattice. From such a crystalline wave function a finite upper bound for E is very easily obtained.[2] Our wave function is "gaseous" in form and describes a perfect gas modified as little as possible by the presence of the interactions. It is interesting that such a wave function continues to behave satisfactorily for values of a as large as b, since $b>\frac{1}{2}a_J$. The question whether there is in fact a transition from a gaseous to a crystalline ground state for any value of $a<a_J$ is one of the famous unsolved problems of statistical mechanics. We are not able to throw any light upon this question.

The coefficient 2π in Eq. (10) is the best possible, by virtue of Eq. (1). Thus the error in the upper

[2] The simplest wave function of this kind gives

$$E<[\sqrt{2}\pi^2\hbar^2N\rho a_J/m][1-(a/a_J)]^{-2}.$$

The essential point of our theorem is that in the first factor on the right of Eq. (10) there appears not a_J but a.

bound is of order a^2 for small a. This means that our wave function must be a reasonably close approximation to the true ground state, representing adequately at least the two-particle correlations.

2. PROOF FOR THE LOWER BOUNDS

In what follows we take $G(u)$ to be any function defined for $0<u<\infty$ and satisfying

$$G(u)\geqslant 0,\quad \int_0^\infty G(u)du=I<\infty. \tag{12}$$

Our proof begins with the following lemma.

Lemma 1.—Let $\psi(r)$ be any function of the space-point r, defined in a region B. Suppose that B is "star-shaped", i.e., if a point P lies in B then B contains the whole of the radius OP. Suppose $\psi(r)=0$ for $r\leq a$. Then

$$\int_B |\mathrm{grad}\psi|^2 d\tau > [3a/I]\int_B G(|r|^3)|\psi|^2 d\tau. \tag{13}$$

Proof of lemma.—Consider the function

$$\phi_0(x)=f(a)-f(x), \tag{14}$$

$$f(x)=\int_x^\infty (s/x)(s-x)G(s^3)ds. \tag{15}$$

This function $\phi_0(x)$ is defined for $a\leq x<\infty$ and satisfies the conditions

$$\phi_0(a)=0,\quad \phi_0'(x)\geq 0, \tag{16}$$

$$0\leq\phi_0(x)\leq f(a)<\int_0^\infty (s^2/a)G(s^3)ds=(I/3a), \tag{17}$$

and

$$-\frac{1}{x}\frac{d^2}{dx^2}(x\phi_0(x))=-G(x^3)=-V(x)\phi_0(x), \tag{18}$$

with

$$V(x)=[G(x^3)/\phi_0(x)]>(3a/I)G(x^3). \tag{19}$$

From Eqs. (16) and (18) it appears that $\phi_0(x)$ is the eigenfunction of the eigenvalue problem

$$-\frac{1}{x}\frac{d^2}{dx^2}[x\phi(x)]=-\lambda V(x)\phi(x),\quad a\leq x<\infty, \tag{20}$$

with boundary condition $\phi(a)=0$, which belongs to the eigenvalue $\lambda=1$. The "potential" $V(x)$ is everywhere positive, and therefore the eigenvalue problem is equivalent to finding the minimum value of the quotient

$$Q=\left[\int_a^\infty x^2|d\phi/dx|^2dx\right]\Big/\left[\int_a^\infty x^2V(x)|\phi|^2dx\right]. \tag{21}$$

The minimum of Q is the lowest eigenvalue λ of Eq. (20). The lowest eigenvalue is necessarily nondegenerate and belongs to the unique eigenfunction of Eq. (20) which has constant sign. But $\phi_0(x)$ is an eigenfunction of constant sign, and therefore $\lambda=1$ is the lowest eigenvalue, and the minimum value of Q is 1.

We have thus proved that for every function $\phi(x)$ with $\phi(a)=0$

$$\int_a^\infty x^2|d\phi/dx|^2dx\geq\int_a^\infty x^2V(x)|\phi|^2dx$$
$$>(3a/I)\int_a^\infty x^2G(x^3)|\phi|^2dx. \tag{22}$$

If $\phi(x)$ is any function defined for $a\leq x\leq b$, and $\phi(a)=0$, then we can extend the definition of $\phi(x)$ by writing $\phi(x)=\phi(b)$ for $x>b$. Thus Eq. (22) gives for any such $\phi(x)$

$$\int_a^b x^2|d\phi/dx|^2dx$$
$$=\int_a^\infty x^2|d\phi/dx|^2dx>(3a/I)\int_a^\infty x^2G(x^3)|\phi|^2dx$$
$$\geq(3a/I)\int_a^b x^2G(x^3)|\phi|^2dx. \tag{23}$$

Now consider the function $\psi(r)$ satisfying the conditions of Lemma 1. For any fixed azimuth of r, $\psi(r)$ is defined in the range $a\leq r\leq b$, where b is the distance from O of the boundary of B in that direction. Writing $\psi(r)$ for $\phi(x)$ in Eq. (23) and integrating over all azimuths, we find

$$\int_B|\partial\psi/\partial r|^2d\tau>[3a/I]\int_B G(|r|^3)|\psi|^2d\tau, \tag{24}$$

from which Eq. (13) immediately follows.

Remark.—It is easy to show by a counter-example that Eq. (13) does not hold for every region B. Some condition on the shape of B is required, though the "star-shaped" condition is probably unnecessarily restrictive.

Proof of Theorem 2.—The ground-state energy of the gas is

$$E=(\hbar^2/2m)\sum_{i=1}^N\int|\mathrm{grad}_i\Psi|^2d\tau_1\cdots d\tau_N, \tag{25}$$

where Ψ is the wave function. Here grad_i means the gradient operator acting upon the coordinates r_i of the ith particle. Consider the positions $(r_2,\cdots,r_N)$ to be temporarily fixed, and regard $\Psi=\Psi(r_1)$ and $R_1=R_1(r_1)$ as functions of the position r_1 alone. Around each point r_j, $j=2,\cdots,N$, there is a region B_j such that r_j is the nearest neighbor of r_1 and $R_1=|r_1-r_j|$ when r_1 is in B_j. The region B_j is convex and therefore star-shaped about the origin r_j. Also $\Psi=0$ when $|r_1-r_j|\leq a$. Hence the conditions of Lemma 1 apply to the function Ψ in the region B_j, with $r=r_1-r_j$. The lemma gives the result

$$\int_{B_j} |\mathrm{grad}_1\Psi|^2 d\tau_1 > [3a/I] \int_{B_j} G(|r_1-r_j|^3)|\Psi|^2 d\tau_1. \quad (26)$$

Summing this over the regions B_j which together fill the box without overlapping, we obtain

$$\int |\mathrm{grad}_1\Psi|^2 d\tau_1 > [3a/I] \int G(R_1^3)|\Psi|^2 d\tau_1. \quad (27)$$

An inequality analogous to Eq. (27) holds for each of the N particles. Adding these inequalities together after integrating over all N variables r_i, we find by Eq. (25)

$$E > [3\hbar^2 a/2mI] \int |\Psi|^2 \left[\sum_{i=1}^{N} G(R_i^3) \right] d\tau_1 \cdots d\tau_N, \quad (28)$$

with I given by Eq. (12). Equation (28) is the fundamental result of this section, from which Theorems 1 and 2 follow easily. Theorem 2 is obtained merely by substituting into Eq. (28) the particular choice

$$G(x) = \delta(x-u) \quad (29)$$

for the function G, and using Eq. (5).

Proof of Theorem 1.—For Theorem 1 we take in Eq. (28) the particular choice

$$G(x) = \max[y-x, 0], \quad I = \tfrac{1}{2}y^2, \quad (30)$$

with the parameter y to be chosen later.

We use the fact that for every configuration of points $(r_1, \cdots, r_N)$ the sum $\sum R_i^3$ cannot exceed a certain upper bound set by purely geometrical considerations. Since the spheres with centers at r_i and radii equal to $\frac{1}{2}R_i$ do not overlap and are all contained in the volume V, we have immediately

$$\sum R_i^3 < (6/\pi)V. \quad (31)$$

A more sophisticated geometrical argument, due to Blichfeldt,[3] gives the stronger result

$$\sum R_i^3 < [15/2\pi\sqrt{2}]V. \quad (32)$$

The proof of Eq. (32) will be found in the Appendix. Substituting Eq. (30) into Eq. (28) and using Eq. (32), we find

$$E > [3\hbar^2 Na/m][y^{-1} - (15/2\pi\sqrt{2})\rho^{-1}y^{-2}]. \quad (33)$$

The most favorable value for y is

$$y = (15/\pi\rho\sqrt{2}), \quad (34)$$

which makes Eq. (33) reduce to Eq. (2). This completes the proof of Theorem 1.

3. PROOF FOR THE UPPER BOUND

The first step is to define the trial wave function. For this purpose we forget about the Bose statistics and consider the positions $(r_1, \cdots, r_N)$ to be attached to N distinguishable particles which are labelled in a definite order from 1 to N. The trial wave function will not be symmetric in the r_i. The expectation value of the Hamiltonian is still a good upper bound to the ground-state energy, because it is known[4] that the ground state of the Bose gas is identical with the ground state of the gas of distinguishable particles.

The trial wave function will be

$$\Psi = \Psi(r_1, \cdots, r_N) = F_1 F_2 \cdots F_N, \quad (35)$$

where F_i is a function of the positions $(r_1, \cdots, r_i)$ only. For each value of i we define

$$t_i = |r_i - r_j|, \quad (36)$$

where r_j is the nearest to r_i among the points $(r_1, \cdots, r_{i-1})$, taking into account the periodic boundary conditions. We write

$$F_i = f(t_i), \quad (37)$$

where $f(t)$ is a function to be specified later. The important properties of f are the following.

$$0 \leq f(t) \leq 1, \quad f'(t) \geq 0, \quad \text{for} \quad 0 \leq t < \infty, \quad (38)$$

$$f(t) = 0 \quad \text{for} \quad 0 \leq t \leq a, \quad (39)$$

$$I = 4\pi \int_0^\infty t^2[1 - f^2(t)]dt < \infty, \quad (40)$$

$$J = 4\pi \int_0^\infty t^2[f'(t)]^2 dt < \infty, \quad (41)$$

$$K = 4\pi \int_0^\infty t^2 f(t) f'(t) dt < \infty. \quad (42)$$

Because of Eq. (39), the wave function Ψ vanishes when any two of the particles are separated by a distance not exceeding a. Thus Ψ represents a possible state of the gas, and the expectation value of the

[3] H. F. Blichfeldt, Math. Ann. **101**, 605 (1929). Blichfeldt was interested in the problem of the maximum density of packing of equal spheres. He proved Eq. (32) for the case in which all the R_i are equal. In this case he showed also that the numerical constant can be improved a little further by a more elaborate construction. However, an improvement much beyond Eq. (32) cannot be hoped for. Empirical evidence suggests the inequality

$$\Sigma R_i^3 \leq \sqrt{2}V, \quad (32a)$$

which holds with equality when the points r_i are vertices of a regular hexagonal lattice. Even if Eq. (32a) could be proved, the effect would only be to replace Theorem 1 by the result

$$E > [3.2^{-5/2}\hbar^2 N\rho a/m],$$

still far away from the conjectured Eq. (9). It seems that a substantial improvement of Theorem 1 can come only from arguments of a dynamical rather than a geometrical character.

[4] The ground state of the Boltzmann gas is necessarily nondegenerate and has a wave function of constant sign. Since the Hamiltonian is symmetric in the particle coordinates, such a nondegenerate wave function must be symmetric. But then this wave function is also the ground state of the Bose gas. For this remark I am indebted to Professor Yang.

Hamiltonian in this state is

$$H=\left(\frac{\hbar^2}{2m}\right)\left[\int\sum_{k=1}^{N}|\mathrm{grad}_k\Psi|^2d\tau_1\cdots d\tau_N\right]\Big/\left[\int|\Psi|^2d\tau_1\cdots d\tau_N\right]. \quad (43)$$

At a point r_k with two equidistant nearest neighbors r_j, $(\mathrm{grad}_k\Psi)$ has a simple discontinuity and Ψ itself is continuous. The integrals in Eq. (43) are therefore convergent and well-defined in spite of the discontinuity.

The physical meaning of the wave function (35) is simple to understand. It describes a state obtained by inserting N particles into the box one at a time. Each new particle takes a wave function which is adjusted to the positions of those particles already present. But the particles added earlier do not adjust themselves to the later additions.

We write

$$\epsilon_{ik}=1,\quad i=k, \quad (44)$$

$$\epsilon_{ik}=-1,\quad t_i=|r_i-r_k|, \quad (45)$$

$$\epsilon_{ik}=0 \text{ otherwise}. \quad (46)$$

Let n_i be the unit vector in the direction of (r_i-r_k) when r_k is the nearest to r_i of the points $(r_1,\cdots,r_{i-1})$. Then

$$\mathrm{grad}_k\Psi=\sum_{i=1}^{N}\Psi F_i^{-1}[\mathrm{grad}_kF_i]=\sum_{i=1}^{N}\Psi\epsilon_{ik}n_iF_i^{-1}f'(t_i). \quad (47)$$

$$\sum_{k=1}^{N}|\mathrm{grad}_k\Psi|^2=|\Psi|^2\sum_i\sum_j\sum_k\epsilon_{ik}\epsilon_{jk}(n_i\cdot n_j)F_i^{-1}F_j^{-1}f'(t_i)f'(t_j)$$
$$\leq|\Psi|^2\sum_i\sum_j\sum_k|\epsilon_{ik}\epsilon_{jk}|F_i^{-1}F_j^{-1}f'(t_i)f'(t_j). \quad (48)$$

We divide the sum (48) into two parts, the first containing terms with $i=j$ and the second with $i\neq j$. When $i=j$ there are exactly two values of k giving nonzero contributions, one with $\epsilon_{ik}=1$ and one with $\epsilon_{ik}=-1$, and the two contributions are equal. When $i<j$ then necessarily $k\leq i<j$. Thus Eq. (48) becomes

$$\sum_{k=1}^{N}|\mathrm{grad}_k\Psi|^2\leq2|\Psi|^2\sum_{i=1}^{N}F_i^{-2}[f'(t_i)]^2+2|\Psi|^2\sum_{k\leq i<j}|\epsilon_{ik}\epsilon_{jk}|F_i^{-1}F_j^{-1}f'(t_i)f'(t_j). \quad (49)$$

Therefore Eq. (43) gives

$$H\leq(\hbar^2/m)[H_1+H_2], \quad (50)$$

$$H_1=\sum_{i=1}^{N}\left[\frac{\int F_1^2\cdots F_{i-1}^2[f'(t_i)]^2F_{i+1}^2\cdots F_N^2d\tau_1\cdots d\tau_N}{\int F_1^2\cdots F_{i-1}^2F_i^2\quad F_{i+1}^2\cdots F_N^2d\tau_1\cdots d\tau_N}\right], \quad (51)$$

$$H_2=\sum_{k\leq i<j}\left[\frac{\int F_1^2\cdots F_{i-1}^2[|\epsilon_{ik}|F_if'(t_i)]F_{i+1}^2\cdots F_{j-1}^2[|\epsilon_{jk}|F_jf'(t_j)]F_{j+1}^2\cdots F_N^2d\tau_1\cdots d\tau_N}{\int F_1^2\cdots F_{i-1}^2F_i^2\quad F_{i+1}^2\cdots F_{j-1}^2F_j^2\quad F_{j+1}^2\cdots F_N^2d\tau_1\cdots d\tau_N}\right]. \quad (52)$$

The fraction (51) would be trivial to estimate if the factors F_{i+1}^2, $\cdots$, F_N^2 did not involve the variable r_i. So we shall set limits upon the possible variation of these factors as r_i varies. Let $i<p\leqslant N$. Let $F_{p,i}$ be the value which F_p would take if the point r_i were omitted from consideration, that is to say

$$F_{p,i}=f(|r_p-r_j|), \quad (53)$$

where r_j is the nearest to r_p of the points $(r_1,\cdots,r_{i-1},r_{i+1},\cdots,r_{p-1})$. Then

$$F_p=\min[F_{p,i},f(|r_p-r_i|)], \quad (54)$$

and so by Eq. (38)

$$F_{p,i}^2f^2(|r_p-r_i|)\leq F_p^2\leq F_{p,i}^2. \quad (55)$$

We set in the numerator of Eq. (51)

$$F_{i+1}^2\cdots F_N^2\leq F_{i+1,i}^2\cdots F_{N,i}^2, \quad (56)$$

while in the denominator

$$F_{i+1}^2\cdots F_N^2\geq F_{i+1,i}^2f^2(|r_{i+1}-r_i|)\cdots F_{N,i}^2f^2(|r_N-r_i|)$$
$$\geq F_{i+1,i}^2\cdots F_{N,i}^2\left[1-\sum_{i+1}^{N}[1-f^2(|r_p-r_i|)]\right]. \quad (57)$$

The factors $F_{p,i}^2$ in Eqs. (56) and (57) are independent of r_i, and so the integration over r_i may be performed at once. We have in the numerator of Eq. (51)

$$\int[f'(t_i)]^2d\tau_i\leq\sum_{j=1}^{i-1}\int[f'(|r_i-r_j|)]^2d\tau_i=(i-1)J, \quad (58)$$

and in the denominator

$$\int\Big[1-\sum_{i+1}^{N}[1-f^2(|r_p-r_i|)]\Big]F_i^2 d\tau_i$$
$$\geq\int\Big[1-\Big(\sum_{i+1}^{N}+\sum_{1}^{i-1}\Big)[1-f^2(|r_p-r_i|)]\Big]d\tau_i$$
$$=V-(N-1)I. \quad (59)$$

The remaining factors are identical in numerator and denominator, and so finally

$$H_1\leq\sum_{i=1}^{N}\frac{(i-1)J}{V-(N-1)I}=\frac{1}{2}\frac{N(N-1)J}{V-(N-1)I}. \quad (60)$$

A similar argument is now applied to Eq. (52). Let $F_{p,ij}$ be the value which F_p would take if both the points r_i and r_j were omitted from consideration. Then

$$F_{p,ij}^2 f^2(|r_p-r_i|)f^2(|r_p-r_j|)\leq F_p^2\leq F_{p,ij}^2. \quad (61)$$

In the numerator of Eq. (52) we set

$$F_{i+1}^2\cdots F_{j-1}^2F_{j+1}^2\cdots F_N^2$$
$$\leq F_{i+1,i}^2\cdots F_{j-1,i}^2F_{j+1,ij}^2\cdots F_{N,ij}^2, \quad (62)$$

and in the denominator

$$F_{i+1}^2\cdots F_{j-1}^2F_{j+1}^2\cdots F_N^2$$
$$\geq F_{i+1,i}^2\cdots F_{j-1,i}^2F_{j+1,ij}^2\cdots F_{N,ij}^2$$
$$\times\Big[1-\Big(\sum_{i+1}^{j-1}+\sum_{i+1}^{N}\Big)[1-f^2(|r_p-r_i|)]\Big]$$
$$\times\Big[1-\sum_{j+1}^{N}[1-f^2(|r_p-r_j|)]\Big]. \quad (63)$$

The integration over r_j is now performed first. In the numerator the factor $|\epsilon_{jk}|$ is zero except when $t_j=|r_j-r_k|$. Therefore

$$\int|\epsilon_{jk}|F_jf'(t_j)d\tau_j$$
$$\leq\int f(|r_j-r_k|)f'(|r_j-r_k|)d\tau_j=K. \quad (64)$$

In the denominator we find

$$\int F_j^2\Big[1-\sum_{j+1}^{N}[1-f^2(|r_p-r_j|)]\Big]d\tau_j$$
$$\geq\int\Big[1-\Big(\sum_{j+1}^{N}+\sum_{1}^{j-1}\Big)[1-f^2(|r_p-r_j|)]\Big]d\tau_j$$
$$=V-(N-1)I. \quad (65)$$

Next we have to perform the summation over k; this gives simply a factor 2 since r_k must be equal either to r_i or to the nearest neighbor of r_i among the points $(r_1,\cdots,r_{i-1})$. After this the r_i integration can be performed, giving in the numerator

$$\int F_if'(t_i)d\tau_i\leq\sum_{1}^{i-1}\int f(|r_i-r_p|)f'(|r_i-r_p|)d\tau_i$$
$$=(i-1)K, \quad (66)$$

and in the denominator

$$\int F_i^2\Big[1-\Big(\sum_{i+1}^{j-1}+\sum_{j+1}^{N}\Big)[1-f^2(|r_p-r_i|)]\Big]d\tau_i$$
$$\geq V-(N-2)I. \quad (67)$$

The remaining factors are identical in numerator and denominator of Eq. (52). Therefore

$$H_2\leq\sum_{i<j}2(i-1)K^2/\{[V-(N-1)I][V-(N-2)I]\}$$
$$=\tfrac{1}{3}N(N-1)(N-2)K^2/$$
$$\{[V-(N-1)I][V-(N-2)I]\}. \quad (68)$$

Putting together Eqs. (50), (60), and (68), we obtain

$$E\leq H\leq\frac{\hbar^2}{2m}\frac{N(N-1)}{V-(N-1)I}\Big[J+\frac{2}{3}\frac{(N-2)K^2}{V-(N-2)I}\Big]$$
$$<\frac{\hbar^2N}{2m}\Big[\Big(\frac{\rho_1J}{1-\rho_1I}\Big)+\frac{2}{3}\Big(\frac{\rho_1K}{1-\rho_1I}\Big)^2\Big], \quad (69)$$

with $\rho_1=[(N-1)/V]$, and I, J, K given by Eqs. (40)–(42). It remains to choose the function $f(x)$ so as to make the right side of Eq. (69) as small as possible. The minimization can be carried through without difficulty, but the details are tedious and will not be discussed here. The upper bound obtained for E in this way is not significantly better than that given by Eq. (10).

We shall content ourselves with proving Eq. (10). This can be done very simply by choosing

$$f(x)=\frac{b}{x}\frac{(x-a)}{(b-a)},\quad a\leq x\leq b; \quad (70)$$

$$f(x)=0,\quad x\leq a;\quad f(x)=1,\quad x\geq b; \quad (71)$$

where b is given by Eq. (11). Then

$$I=(4/3)\pi ab^2,\quad \rho_1I=(a/b), \quad (72)$$

$$J=4\pi ab/(b-a), \quad (73)$$

$$K=[4\pi b^2a/(b-a)^2][b-a-a\ln(b/a)]<4\pi ab, \quad (74)$$

and so Eq. (69) reduces directly to Eq. (10).

Remarks.—With the best possible $f(x)$, the first factor in Eq. (10) remains unchanged, and only the coefficients of (a/b) in the second factor are somewhat improved. But from the calculations of Lee and Yang[1] it is known that as $a\to 0$ the correct form of the second factor in Eq. (10) should be $[1+O(a/b)^{\frac{3}{2}}]$. Thus the terms linear in (a/b) ought not to be present and arise from the crudeness of our analysis; the coefficients of these terms do not possess any physical significance.

It is an interesting question, whether an exact evaluation of the expectation value of the Hamiltonian for the trial wave function (35) would give an upper bound for E with an error of relative order $(a/b)^{\frac{3}{2}}$ or smaller. It is our belief that this is so, and that the terms of order (a/b) could be removed by a more careful calculation with the same wave-function.

I wish to thank Professors Lee and Yang for stimulating my interest in this problem, and for many helpful discussions.*

APPENDIX. PROOF OF EQ. (32)

We prove that Eq. (32) holds for any configuration of points $(\mathbf{r}_1,\cdots,\mathbf{r}_N)$ contained in the volume V. Here R_i is the distance from $\mathbf{r}_i$ to its nearest neighbor among the $\mathbf{r}_j$, taking into account the periodic boundary conditions.

We consider the function

$$F(\mathbf{r})=\sum_{i=1}^{N} f_i(\mathbf{r}), \tag{75}$$

$$f_i(\mathbf{r})=\max[1-2R_i^{-2}(\mathbf{r}-\mathbf{r}_i)^2,\,0]. \tag{76}$$

Let the point $\mathbf{r}$ be fixed, and let the m points $\mathbf{r}_i$ for which $f_i(\mathbf{r})>0$ be temporarily labeled $(\mathbf{r}_1,\cdots,\mathbf{r}_m)$. For each pair $(i\neq j)$ we have

$$(\mathbf{r}_i-\mathbf{r}_j)^2=(\mathbf{r}-\mathbf{r}_i)^2+(\mathbf{r}-\mathbf{r}_j)^2 -2(\mathbf{r}-\mathbf{r}_i)(\mathbf{r}-\mathbf{r}_j)\geq R_i^2. \tag{77}$$

Therefore

$$0\leq \Big|\sum_{i=1}^{m} R_i^{-2}(\mathbf{r}-\mathbf{r}_i)\Big|^2$$

$$=\sum_{i=1}^{m} R_i^{-4}(\mathbf{r}-\mathbf{r}_i)^2+\sum_{i\neq 1} R_i^{-2}R_j^{-2}(\mathbf{r}-\mathbf{r}_i)(\mathbf{r}-\mathbf{r}_j),$$

$$\leq \sum_{i=1}^{m} R_i^{-4}(\mathbf{r}-\mathbf{r}_i)^2+\frac{1}{2}\sum_{i\neq j} R_i^{-2}R_j^{-2}$$

$$\times[(\mathbf{r}-\mathbf{r}_i)^2+(\mathbf{r}-\mathbf{r}_j)^2-R_i^2]=\Big[\sum_{i=1}^{m} R_i^{-2}\Big] \times\Big[\sum_{j=1}^{m} R_j^{-2}(\mathbf{r}-\mathbf{r}_j)^2-\frac{1}{2}(m-1)\Big], \tag{78}$$

and hence

$$F(\mathbf{r})=\sum_{j=1}^{m}[1-2R_j^{-2}(\mathbf{r}-\mathbf{r}_j)^2]\leq m-(m-1)=1. \tag{79}$$

From Eq. (79) it follows that

$$\int F(\mathbf{r})d\tau\leq V. \tag{80}$$

On the other hand, Eq. (76) gives

$$\int F(\mathbf{r})d\tau=\sum_{i=1}^{N}\int f_i(\mathbf{r})d\tau$$

$$=\sum_{i=1}^{N}\int_0^{R_i/\sqrt{2}}[1-2R_i^{-2}x^2]4\pi x^2dx$$

$$=\left(\frac{2\pi\sqrt{2}}{15}\right)\sum_{i=1}^{N} R_i^3. \tag{81}$$

Equations (80) and (81) together imply Eq. (32).

* *Note added in proof.*—R. Jastrow [Phys. Rev. 98, 1479 (1955)], and R. B. Dingle [Phil. Mag. 40, 573 (1949)], have calculated the ground state energy using a trial wave function of the form $\Pi f(\mathbf{r}_i-\mathbf{r}_j)$, the product being taken over all pairs of particles. This wave function is undoubtedly a closer approximation to the true ground state than our Eq. (35) which takes into account the interaction only between pairs of nearest neighbors. However Jastrow is not able with his wave function to obtain a rigorous upper bound to the energy. His expression for the energy is a series of cluster integrals which he is obliged to break off without controlling the error. The purpose of the present paper was to show that the "nearest-neighbor" type of wave function permits a new approach to the description of many-body systems with strong interactions, in which the familiar difficulties associated with cluster-integral expansions do not arise.