n_3', and n_4' as α_0, β_0 and γ_0 are of n_1, n_2, n_3, and n_4. Because of the symmetry of the summand with respect to the interchanges of suffices $1 \leftrightarrow 2$, $3 \leftrightarrow 4$, the foregoing sum would exactly cancel with the second part of the quadruple sum in Σ. We are thus left with only the double sum in (134) which is found to be

$$-4(m+m^*)^{-3/2} \sum_{n_1,n_3=1}^{\infty} (n_1 n_3)^{-2} \left(n_1 n_3 - \frac{m n_1 + m^* n_3}{m+m^*} \right)^{1/2} z^{n_1} z^{*n_3}. \tag{136}$$

Introducing the constants appearing in (126), this gives

$$-4\bar{a}^2 m m^* (m+m^*)^{1/2} (2\pi\beta)^{-5/2} \sum_{r,s=1}^{\infty} (rs)^{-2} \left(rs - \frac{mr + m^* s}{m+m^*} \right)^{1/2} z^r z^{*s}. \tag{137}$$

The final result for the integral I is then equal to the sum of (133) and (137).

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Quantum Cell Model for Bosons

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An approach is presented toward validating the assumption that the ground state of bosons with repulsive interactions at low densities is characterized by macroscopic occupation of the zero momentum level. We use a cell model which affords a simple description of the high-density region, where fluctuations in number density are small and where no single-particle level is macroscopically occupied. As the density decreases, fluctuations increase, and we reach a critical density at which the small fluctuation approximation becomes unstable with respect to plane wave states of zero momentum. At this critical density, the single-particle energy gap disappears, and the dependence of excitation energy on momentum changes from quadratic to linear, for small values of momentum.

I. INTRODUCTION

THE model of N hard-sphere bosons at low densities has been very successful in predicting many of the physical properties of a superfluid.[1] Of significance in theoretical treatments is the role played by the assumption that in the presence of the repulsive interactions a finite fraction of particles occupy the state with zero linear momentum. In the second quantized formulation of the model, this assumption facilitates reduction of the Hamiltonian operator from quadrilinear to quadratic form in plane wave creation and destruction operators.[1] In a configurational-space approach, it enables one to calculate the effects of interaction using the ring integrals of Mayer cluster theory.[2]

This assumption regarding a macroscopically occupied level is physically plausible for repulsive interactions at low particle densities. Moreover, it provides a self-consistent theoretical development, that is, once it is invoked, the theory shows that the interactions do not destroy the macroscopic single level occupation. However, the validity of the assumption has never been proved.

Our aim here is to attempt to indicate with a simplified model how the condensation in momentum space may result spontaneously from the theory without having to assume it at the outset. Such is the state of affairs in the treatment of thermodynamic properties characterizing an ideal Bose gas.[3] There, at sufficiently high temperatures, no single-particle level is macroscopically occupied. As the temperature is decreased below a critical value, the requirement concerning a fixed number of particles comprising the system forces a finite fraction of the particles to occupy the lowest momentum level. One thus obtains a complete description of the ideal gas of bosons in both the region of no macroscopic occupation of a single-particle level (normal region) and the region of macroscopic occupation of the single-particle zero momentum level (superfluid region). It would, of course, be pleasing to have the same complete description for bosons with repulsive interactions. We have not developed such an inclusive treatment in this work, but rather have observed the ground state of the system starting from

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high densities (normal region) and proceeding to smaller densities, until the appearance of an instability in the theory.

We treat the system of bosons with repulsive interactions by using a cell model which affords a simple description of the high-density region in which the particles are well localized by the repulsive interactions. In a representation which diagonalizes the cell occupation numbers, the potential energy operator is diagonal, while the kinetic energy operator has off-diagonal terms which cause transitions of particles from one cell to another. At high densities these transitions are rare events so that we can develop an approximation for small fluctuations in occupation numbers about the average number. Under these circumstances, the momentum distribution of the particles is a smoothly varying function of momentum, with no single level macroscopically occupied. The single-particle excitation spectrum exhibits an energy gap, and a quadratic dependence of excitation energy on momentum. As the density decreases, the particle wanderings become greater, and fluctuations increase. Finally, at a low, critical density, the small fluctuation approximation becomes unstable with respect to formation of states where particles are free to wander unrestricted over the entire volume, i.e., plane wave states of zero momentum. At this critical density, the energy gap disappears, and the single-particle energy has a linear dependence on momentum, for small values of momentum. For densities less than this critical density, one would have to replace the small fluctuation approximation by one which allows for the large fluctuations in number density accompanying the greatly increased occupation of the zero momentum state.

In Sec. II, we develop the cell model Hamiltonian, and show that it is capable of reproducing several well-known approximations.

In Sec. III, the description of the ground state as one of limited fluctuations is made, using Green's function techniques, and the instability at low densities is demonstrated.

II. FORMULATION OF THE CELL MODEL

A system of spinless, nonrelativistic boson particles is considered to be enclosed in a large box. Both the number N of interacting particles and the volume Ω of the box are assumed to be so large that all effects which are small in the limit $N\rightarrow\infty$ and $\Omega\rightarrow\infty$ can be neglected, the particle density $\rho=N/\Omega$ remaining finite.

In the formalism of second quantization, the Hamiltonian operator for such a system is represented by

$$H=-\frac{\hbar^2}{2m}\int\psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r})d\tau + \frac{1}{2}\int\psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r})U(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r})\psi(\mathbf{r}')d\tau d\tau', \quad (1)$$

where $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$ are, respectively, creation and destruction operators for a particle positioned at $\mathbf{r}$, and $U(\mathbf{r}-\mathbf{r}')$ is the interaction potential for particles at $\mathbf{r}$ and $\mathbf{r}'$. The number operator representing the total number of particles is

$$N=\int\psi^\dagger(\mathbf{r})\psi(\mathbf{r})d\tau, \quad (2)$$

and the commutation relations for bosons are

$$\begin{aligned}&[\psi(\mathbf{r}),\psi(\mathbf{r}')]=[\psi^\dagger(\mathbf{r}),\psi^\dagger(\mathbf{r}')]=0,\\&[\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')]=\delta(\mathbf{r}-\mathbf{r}').\end{aligned} \quad (3)$$

For systems of low density, the field operator $\psi(\mathbf{r})$ is customarily expanded in a complete set of plane wave states. Since the system of interest here is one of close packing, an expansion of $\psi(\mathbf{r})$ in a localized set of functions is desirable. Accordingly, the box of boson particles is divided into cells of size τ equal to the specific volume $1/\rho$. The field operator is expanded in a complete orthogonal set of functions $f(\mathbf{r}-\mathbf{r}_j)$ centered on the jth cell,

$$\psi(\mathbf{r})=\rho^{1/2}\textstyle\sum_{\mathbf{r}_j} b_{\mathbf{r}_j}f(\mathbf{r}-\mathbf{r}_j). \quad (4)$$

We choose Kronecker δ functions for the orthogonal set,

$$\begin{aligned}\delta_{\mathbf{r},\mathbf{r}_j}&=1, \text{ if } \mathbf{r} \text{ is in cell centered on } \mathbf{r}_j,\\&=0, \text{ otherwise.}\end{aligned} \quad (5)$$

The field operator is thus assigned a constant amplitude throughout a cell, resulting in the loss of some detail regarding the fine structure of the model. However, the properties sensitive to wavelengths, long compared to a cell dimension, should still be obtainable with precision. The field operator $\psi(\mathbf{r})$ now has the form

$$\psi(\mathbf{r})=\rho^{1/2}\textstyle\sum_{\mathbf{r}_j} b_{\mathbf{r}_j}\delta_{\mathbf{r},\mathbf{r}_j} \quad (6)$$

as opposed to the usual Fourier decomposition into plane waves. From Eq. (6) follows the commutation relations for the operators $b_{\mathbf{r}_j}$,

$$\begin{aligned}&[b_{\mathbf{r}_m},b_{\mathbf{r}_k}]=[b_{\mathbf{r}_m}^\dagger,b_{\mathbf{r}_k}^\dagger]=0,\\&[b_{\mathbf{r}_m},b_{\mathbf{r}_k}^\dagger]=\delta_{\mathbf{r}_m,\mathbf{r}_k}.\end{aligned} \quad (7)$$

The number operator of Eq. (2) becomes, in terms of these new operators,

$$N=\textstyle\sum_{\mathbf{r}_j} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}=\sum_{\mathbf{r}_j} n_{\mathbf{r}_j}, \quad (8)$$

where $n_{\mathbf{r}_j}=b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}$ is the occupation number of the cell j.

Equation (6) is now introduced into the Hamiltonian operator of Eq. (1) to express the latter in the new operator notation. The kinetic energy operator T of Eq. (1) is

$$T=-\frac{\hbar^2}{2m}\int\psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r})d\tau. \quad (9)$$

A finite difference approximation is adopted for the operator $\nabla^2 b_{\mathbf{r}_j}\delta_{\mathbf{r},\mathbf{r}_j}$. In a three-dimensional model with

a simple cubic lattice, the approximation is

$$\nabla^2 b_{\mathbf{r}_j}\delta_{\mathbf{r},\mathbf{r}_j} \cong (1/r_0^2)[-6b_{\mathbf{r}_j}\delta_{\mathbf{r},\mathbf{r}_j}+\textstyle\sum_{\mathbf{r}'} b_{\mathbf{r}_j}\delta_{\mathbf{r},\mathbf{r}_j+\mathbf{r}'}], \quad (10)$$

where $\mathbf{r}'$ extends over the six nearest neighbors to $\mathbf{r}_j$, and where r_0^3 is the volume τ of a cell, which is the reciprocal of the particle density ρ. With this finite difference approximation the kinetic energy operator of Eq. (9) becomes

$$T=3\frac{\hbar^2}{m}\rho^{2/3}\sum_{\mathbf{r}_j} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}-\frac{\hbar^2}{2m}\rho^{2/3}\sum_{\mathbf{r}_j,\mathbf{r}'} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j+\mathbf{r}'}. \quad (11)$$

Reference to Eq. (8) shows that the first term appearing on the right in Eq. (11) above is simply the sum of $n_{\mathbf{r}_j}$ times a zero-point kinetic energy for localization of a particle in a cell. The second term on the right side of Eq. (11)—the off-diagonal element—represents the drifting of particles into neighboring cells. This latter term affects a decrease in the kinetic energy from its value for localized particles, an understandable result since the shifting of particles spreads out the wave function which implies a reduced kinetic energy.

A second step in the reduction of Eq. (1) to its equivalent representation in terms of the cell creation and destruction operators is the description of the potential energy operator V. Substitution of Eq. (6) and simplification leads to

$$V=\tfrac{1}{2}\rho^2\sum_{\mathbf{r}_j}\sum_{\mathbf{r}_k} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_k}^\dagger b_{\mathbf{r}_j} b_{\mathbf{r}_k}\int_{\mathbf{r}\in j,\mathbf{r}'\in k}\int U(\mathbf{r}-\mathbf{r}')d\tau d\tau'. \quad (12)$$

We rewrite this as

$$V=\tfrac{1}{2}\rho U_0\sum_{\mathbf{r}_j} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j} b_{\mathbf{r}_j} +\tfrac{1}{2}\rho\sum_{\substack{\mathbf{r}_j\mathbf{r}_k\\ \mathbf{r}_j\neq\mathbf{r}_k}}\sum U_{\mathbf{r}_j,\mathbf{r}_k} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j} b_{\mathbf{r}_k}^\dagger b_{\mathbf{r}_k}, \quad (13)$$

where the effective interaction potentials U_0 and U_{r_j,r_k} are defined as

$$\begin{aligned} U_0&=\rho\int\int U(\mathbf{r}-\mathbf{r}')d\tau d\tau', \quad \mathbf{r},\ \mathbf{r}' \text{ in one cell,}\\ U_{\mathbf{r}_j,\mathbf{r}_k}&=\rho\int\int U(\mathbf{r}-\mathbf{r}')d\tau d\tau', \quad \mathbf{r} \text{ in cell } j,\\ &\qquad\qquad \mathbf{r}' \text{ in cell } k. \end{aligned} \quad (14)$$

Equations (14) impose a limitation to integrable potentials. The inclusion in the function $f(\mathbf{r}-\mathbf{r}_j)$ appearing in Eq. (4) of a local function for each cell would obviate this restriction. Mathematical expediency dictated the approach taken herein. Using the commutation relations of Eq. (7) we can write the potential energy operator V in the form

$$V=\tfrac{1}{2}\rho U_0\sum_{\mathbf{r}_j} n_{\mathbf{r}_j}(n_{\mathbf{r}_j}-1)+\tfrac{1}{2}\rho\sum_{\substack{\mathbf{r}_j\mathbf{r}_k\\ \mathbf{r}_j\neq\mathbf{r}_k}}\sum n_{\mathbf{r}_j}n_{\mathbf{r}_k}U_{\mathbf{r}_j,\mathbf{r}_k}. \quad (15)$$

In the following work, the term involving $U_{\mathbf{r}_j,\mathbf{r}_k}$ in Eqs. (13) or (15) will be neglected on the following basis. Since physically realizable potentials are of relatively short range, the integration over cells in the second of Eqs. (14) will yield a relatively insignificant contribution as compared with that given by the first of Eqs. (14). Combining the principal part of Eq. (13) with Eq. (11) gives the Hamiltonian operator in the following form:

$$H=6K\sum_{\mathbf{r}_j} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}-K\sum_{\mathbf{r}_j,\mathbf{r}'} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j+\mathbf{r}'} +\tfrac{1}{2}\rho U_0\sum_{\mathbf{r}_j} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j} b_{\mathbf{r}_j}, \quad (16)$$

where $K=\hbar^2\rho^{2/3}/2m$. This is the Hamiltonian we use in our subsequent work.

A brief qualitative discussion of the foregoing Hamiltonian will now be presented. For repulsive interactions at a high density ρ, we have the inequality

$$\rho U_0 \gg \hbar^2\rho^{2/3}/2m.$$

Thus, particles are inhibited from shifting about, and, as expected, a "locked-in" behavior ensues. The ground state of the system then corresponds to one particle per cell with little or no wanderings. In the opposite extreme of low densities we have the reverse inequality

$$\rho U_0 \ll \hbar^2\rho^{2/3}/2m,$$

and the kinetic energy portion of the Hamiltonian predominates. Now there are significant fluctuations in the cell occupation number about the average value of one particle for the ground state, and large particle wanderings occur. If U_0 is allowed to become negative there will again be large fluctuations in particle numbers in each cell and, unless the fluctuations are limited, the whole system collapses.

It is of interest to conclude the cell model development by deriving several known results using the Hamiltonian operator in Eq. (16). First we treat the case of free particles, $U_0=0$. The Hamiltonian in Eq. (16) becomes in this case

$$H=6K\textstyle\sum_{\mathbf{r}_i} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}-K\sum_{\mathbf{r}_j}\sum_{\mathbf{r}'} b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j+\mathbf{r}'}. \quad (17)$$

A canonical transformation is made which diagonalizes the Hamiltonian, namely,

$$b_{\mathbf{r}_j}=N^{-1/2}\textstyle\sum_{\mathbf{q}} a_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}_j}. \quad (18)$$

Then Eq. (16) reads

$$H=2K\textstyle\sum_{\mathbf{q}}(3-\frac{1}{2}\sum_{\mathbf{r}'} e^{i\mathbf{q}\cdot\mathbf{r}'})a_{\mathbf{q}}^\dagger a_{\mathbf{q}}=\sum_{\mathbf{q}}\epsilon_{\mathbf{q}}a_{\mathbf{q}}^\dagger a_{\mathbf{q}}. \quad (19)$$

Since it follows from Eq. (18) that $a_{\mathbf{q}}^\dagger$ and $a_{\mathbf{q}}$ are creation and destruction operators, respectively, for plane waves of momentum $\mathbf{q}$, $\epsilon_{\mathbf{q}}$ is the corresponding energy,

$$\epsilon_{\mathbf{q}}=2K(3-\cos q_x r_0-\cos q_y r_0-\cos q_z r_0). \quad (20)$$

For low momentum, corresponding to wavelengths long

compared with a cell dimension r_0, expansion of the cosine function yields

$$\epsilon_q=(\hbar^2\rho^{2/3}/2m)q^2r_0^2=\hbar^2q^2/2m. \tag{21}$$

Equation (21) represents a known result correct for free particles. It is noted that the appearance of the trigonometric function in Eq. (20) is a direct consequence of the cell-type model which we have employed.

Next, we calculate the expectation value for the potential energy, $\langle V\rangle$, for the ground state at low density, where from Eq. (15)

$$\langle V\rangle=\tfrac{1}{2}\rho U_0\sum_{\mathbf{r}_j}\langle n_{\mathbf{r}_j}(n_{\mathbf{r}_j}-1)\rangle$$
$$=\tfrac{1}{2}N\rho U_0[\langle n_{\mathbf{r}_1}^2\rangle-1/[\langle n_{\mathbf{r}_1}^2\rangle-1]. \tag{22}$$

To compute $\langle n_{\mathbf{r}_1}^2\rangle$, one expresses the number of particles in a cell by the Poisson distribution function. Hence, the probability that exactly $n_{\mathbf{r}_1}$ particles are contained in the cell centered about $\mathbf{r}_1$ is

$$P(n_{\mathbf{r}_1})=(1/e)(1/n_{\mathbf{r}_1}!). \tag{23}$$

Then

$$\langle n_{\mathbf{r}_1}^2\rangle=\sum_{n_{\mathbf{r}_1}=0}^{\infty}n_{\mathbf{r}_1}^2P(n_{\mathbf{r}_1})=2. \tag{24}$$

With reference to Eq. (14) one can express $\langle V\rangle$ as follows:

$$\langle V\rangle=\tfrac{1}{2}N\rho U_0=\tfrac{1}{2}N\rho^2\int\int U(\mathbf{r}-\mathbf{r}')d\tau d\tau'. \tag{25}$$

For relatively short-range potentials, one can integrate over the volume τ' to obtain

$$\langle V\rangle=\tfrac{1}{2}N\rho\int U(q)d\tau_q, \tag{26}$$

where $q=|\mathbf{r}-\mathbf{r}'|$. The above result is identical with that obtained from first order perturbation theory in the low-density region.[1]

Lastly, for low densities the Hamiltonian of Eq. (16) can be approximated and subsequently diagonalized to yield the energy of low momentum excitations which correspond to sound waves or phonons, the results agreeing with those given in reference 1. One writes as a first approximation in this case

$$b_{\mathbf{r}_j}=1+\xi_{\mathbf{r}_j}, \tag{27}$$

whereupon the Hamiltonian assumes the quadratic form (details of the calculation are presented in Appendix A)

$$H=\tfrac{1}{2}N\rho U_0+K\sum_{\mathbf{r}_j}(6\xi_{\mathbf{r}_j}^\dagger\xi_{\mathbf{r}_j}-\sum_{\mathbf{r}'}\xi_{\mathbf{r}_j}^\dagger\xi_{\mathbf{r}_j+\mathbf{r}'})$$
$$+\tfrac{1}{2}\rho U_0\sum_{\mathbf{r}_j}(\xi_{\mathbf{r}_j}^\dagger\xi_{\mathbf{r}_j}^\dagger+2\xi_{\mathbf{r}_j}^\dagger\xi_{\mathbf{r}_j}+\xi_{\mathbf{r}_j}\xi_{\mathbf{r}_j}). \tag{28}$$

Since the ξ's are assumed small with respect to unity, products of three or more of these operators have been neglected. Introducing the plane wave representation

$$\xi_{\mathbf{r}_j}=N^{-1/2}\sum_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}_j}, \tag{29}$$

one finds that Eq. (28) reads

$$H=\tfrac{1}{2}N\rho U_0+\sum_{\mathbf{k}}\left[\left(\frac{\hbar^2k^2}{2m}+\rho U_0\right)a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right.$$
$$\left.+\tfrac{1}{2}\rho U_0(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger+a_{\mathbf{k}}a_{-\mathbf{k}})\right]. \tag{30}$$

The same approximation for low momentum has been used in obtaining Eq. (30) as that previously employed in the free-particle case. The Hamiltonian of Eq. (30) is now identical to that used in reference 1 and can be diagonalized with the Bogoliubov transformation

$$a_{\mathbf{k}}=u_k\eta_{\mathbf{k}}+v_k\eta_{-\mathbf{k}}^\dagger, \tag{31}$$

where $u_k^2-v_k^2=1$ in order that the new operators $\eta_{\mathbf{k}}$, $\eta_{\mathbf{k}}^\dagger$ obey the same commutation rules as the old ones. This process yields the familiar expression for the energy of the elementary excitations or quasi-particles

$$\epsilon_k=[(\hbar^2k^2/2m)(\hbar^2k^2/2m+2\rho U_0)]^{1/2}. \tag{32}$$

III. LOCALIZED SOLUTIONS AND INSTABILITY

We now resort to the Green's function technique and terminate the hierarchy of coupled Green's function equations of motion on the basis that only small fluctuations occur in the cell occupation number about its average value of unity.

The one-particle Green's function is defined as

$$G_1(\mathbf{r}_j,t;\mathbf{r}_k,t')=-i\langle Tb_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^\dagger(t')\rangle, \tag{33}$$

where T indicates a time ordered product of operators, as follows:

$$Tb_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^\dagger(t')=\theta(t-t')b_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^\dagger(t')$$
$$+\theta(t'-t)b_{\mathbf{r}_k}^\dagger(t')b_{\mathbf{r}_j}(t), \tag{34}$$

in which

$$\theta(t)=1 \quad \text{if} \quad t>0,$$
$$=0 \quad \text{if} \quad t<0. \tag{35}$$

We take the expectation value indicated in Eq. (33) with respect to the true ground state of the system. The equation of motion for $G_1(\mathbf{r}_j,t;\mathbf{r}_k,t')$ derivable from Eqs. (33) and (34) is

$$i\frac{d}{dt}G_1(\mathbf{r}_j,t;\mathbf{r}_k,t')=\delta_{\mathbf{r}_j,\mathbf{r}_k}\delta(t-t')$$
$$-\frac{i}{\hbar}\langle T[b_{\mathbf{r}_j}(t),H(t)]b_{\mathbf{r}_k}^\dagger(t')\rangle, \tag{36}$$

where we have used the equation of motion for the operator $b_{\mathbf{r}_j}(t)$,

$$i\hbar(db_{\mathbf{r}_j}/dt)=[b_{\mathbf{r}_j},H]. \tag{37}$$

The commutator of $b_{\mathbf{r}_j}$ and H is obtained, using Eq. (16), as

$$[b_{\mathbf{r}_j},H]=K(6b_{\mathbf{r}_j}-\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'})+\rho U_0b_{\mathbf{r}_j}^\dagger b_{\mathbf{r}_j}b_{\mathbf{r}_j}, \tag{38}$$

so that G_1 satisfies the equation (hereafter we put $\hbar=1$)

$$\left(i\frac{d}{dt}-6K\right)G_1(\mathbf{r}_j,t;\mathbf{r}_k,t')$$
$$=\delta_{\mathbf{r}_j,\mathbf{r}_k}\delta(t-t')-K\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',t;\mathbf{r}_k,t')$$
$$-i\rho U_0\langle Tb_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle. \quad (39)$$

We now define a two-particle Green's function by the equation

$$G_2(\mathbf{r}_j,t;\mathbf{r}_k,t')=-i\langle Tb_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle. \quad (40)$$

This Green's function, which depends only on the time difference $t-t'$, is simpler than the commonly used multiple-time two-particle Green's function[4] and yet appears to contain adequate information about the physical properties of the model. Such "double-time" Green's functions have been discussed by Zubarev.[5] In terms of the two-particle function, Eq. (39) for G_1 reads

$$\left(i\frac{d}{dt}-6K\right)G_1(\mathbf{r}_j,t;\mathbf{r}_k,t')$$
$$=\delta_{\mathbf{r}_j,\mathbf{r}_k}\delta(t-t')-K\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',t;\mathbf{r}_k,t')$$
$$+\rho U_0G_2(\mathbf{r}_j,t;\mathbf{r}_k,t'). \quad (41)$$

The expectation value for the ground-state energy can be expressed in terms of the functions G_1 and G_2 as follows:

$$\langle H\rangle=\lim_{t'\to t+}i\sum_{\mathbf{r}_j}\{K[6G_1(\mathbf{r}_j,t;\mathbf{r}_j,t')$$
$$-\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',t;\mathbf{r}_j,t')]+\tfrac{1}{2}\rho U_0G_2(\mathbf{r}_j,t;\mathbf{r}_j,t')\}. \quad (42)$$

Since all cells are equivalent, the summations over all cells in Eq. (42) can be replaced by values of G_1 and G_2 in any one cell times the number of cells. From our choice of cell size $=1/\rho$, the specific volume, the number of cells is equal to N, the number of particles. Then the ground-state energy per particle is given by

$$\frac{\langle H\rangle}{N}=\lim_{t'\to t+}\{K[6G_1(\mathbf{r}_j,t;\mathbf{r}_j,t')$$
$$-\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',t;\mathbf{r}_j,t')]+\tfrac{1}{2}\rho U_0G_2(\mathbf{r}_j,t;\mathbf{r}_j,t')\}. \quad (43)$$

We require the equation satisfied by G_2 which follows from

$$i\frac{d}{dt}G_2(\mathbf{r}_j,t;\mathbf{r}_k,t')=\frac{d}{dt}\langle Tb_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle. \quad (44)$$

Let

$$A_{\mathbf{r}_j}(t)=b_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t). \quad (45)$$

Then G_2 satisfies the equation

$$i(d/dt)G_2(\mathbf{r}_j,t;\mathbf{r}_k,t')=(d/dt)\langle TA_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle$$
$$=\delta(t-t')\langle[A_{\mathbf{r}_j}(t),b_{\mathbf{r}_k}^{\dagger}(t')]\rangle$$
$$-i\langle T[A_{\mathbf{r}_j}(t),H(t)]b_{\mathbf{r}_k}^{\dagger}(t')\rangle. \quad (46)$$

For the commutator of $A_{\mathbf{r}_j}$ with H, we find

$$[A_{\mathbf{r}_j},H]=(6K+\rho U_0)b_{\mathbf{r}_j}^{\dagger}b_{\mathbf{r}_j}b_{\mathbf{r}_j}-2Kb_{\mathbf{r}_j}^{\dagger}b_{\mathbf{r}_j}\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}$$
$$+K\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}^{\dagger}b_{\mathbf{r}_j}b_{\mathbf{r}_j}+\rho U_0b_{\mathbf{r}_j}^{\dagger}b_{\mathbf{r}_j}^{\dagger}b_{\mathbf{r}_j}b_{\mathbf{r}_j}b_{\mathbf{r}_j}, \quad (47)$$

while for the commutator of $A_{\mathbf{r}_j}$ with $b_{\mathbf{r}_k}(t')$ we have

$$[A_{\mathbf{r}_j}(t),b_{\mathbf{r}_k}^{\dagger}(t')]=2b_{\mathbf{r}_j}^{\dagger}b_{\mathbf{r}_j}\delta_{\mathbf{r}_j\mathbf{r}_k}\delta(t-t'), \quad (48)$$

from which

$$\langle[A_{\mathbf{r}_j}(t),b_{\mathbf{r}_k}^{\dagger}(t')]\rangle=2\langle n_{\mathbf{r}_j}\rangle\delta_{\mathbf{r}_j,\mathbf{r}_k}\delta(t-t')$$
$$=2\delta_{\mathbf{r}_j,\mathbf{r}_k}\delta(t-t'). \quad (49)$$

For G_2 we may now write the equation

$$\left(i\frac{d}{dt}-6K-\rho U_0\right)G_2(\mathbf{r}_j,t;\mathbf{r}_k,t')=2\delta_{\mathbf{r}_j,\mathbf{r}_k}\delta(t-t')$$
$$+2Ki\langle Tb_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}(t)\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle$$
$$-iK\langle T\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}^{\dagger}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle$$
$$-i\rho U_0\langle Tb_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle. \quad (50)$$

Since only two time variables have been employed herein, Eq. (50) for G_2 differs somewhat in form from the corresponding equation involving the customary multiple-time two-particle Green's function.[4] It has, however, the familiar characteristic of coupling G_2 to a "three-particle" Green's function, represented by the last term on the right side of Eq. (50).

We now terminate and simplify the hierarchy of equations, of which Eqs. (41) and (50) are the first two, by using our assumption that the repulsive interaction dominates the kinetic energy, $\rho U_0\gg K$. Consistent with the concomitant implication that there occurs, for the ground state, only small fluctuations in occupation number about the average value of unity, we may neglect the last term on the right side of Eq. (50), which involves the destruction of three particles in the cell centered on $\mathbf{r}_j$. This means that the occupation number of particles in any particular cell is prohibited from exceeding two. In addition, we introduce the following approximations for the two remaining expectation values on the right-hand side of Eq. (50)[6]:

$$\langle Tb_{\mathbf{r}_j}^{\dagger}(t)b_{\mathbf{r}_j}(t)\sum_{\mathbf{r}'}{}'b_{\mathbf{r}_j+\mathbf{r}'}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle$$
$$\cong\langle b_{\mathbf{r}_j}^{\dagger}b_{\mathbf{r}_j}\rangle\langle T\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle$$
$$\cong\langle T\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle, \quad (51)$$

$$\langle T\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}^{\dagger}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle$$
$$\cong\langle\sum_{\mathbf{r}'}b_{\mathbf{r}_j+\mathbf{r}'}^{\dagger}b_{\mathbf{r}_j}\rangle\langle Tb_{\mathbf{r}_j}(t)b_{\mathbf{r}_k}^{\dagger}(t')\rangle. \quad (52)$$

[4] P. D. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).
[5] D. N. Zubarev, Soviet Phys.—Uspekhi **3**, 320 (1960).

[6] To advance the justification for these approximations beyond the intuitive level, we note that they lead to the same ground state energy as that derived by a perturbation approach (see concluding paragraph, Appendix B).

These approximations allow us to rewrite Eq. (50) as

$$\left[i\frac{d}{dt}-6K-\rho U_0\right]G_2(\mathbf{r}_j,t;\mathbf{r}_k,t')$$
$$=2\delta_{\mathbf{r}_j,\mathbf{r}_k}\delta(t-t')-2K\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',t;\mathbf{r}_k,t')$$
$$+K\sum_{\mathbf{r}'}\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle G_1(\mathbf{r}_j,t;\mathbf{r}_k,t'). \quad (53)$$

The effect of the off-diagonal terms in the kinetic energy operator is reflected only in the two last terms on the right side of Eq. (53). Equations (41) and (53) form a pair of coupled differential equations for G_1 and G_2 which can easily be solved. First introduce the spectral resolutions

$$G_m(\mathbf{r}_j,t;\mathbf{r}_k,t')=(2\pi)^{-1}\int_{-\infty}^{\infty}G_m(\mathbf{r}_j,\mathbf{r}_k,\omega)e^{-i\omega(t-t')}d\omega,$$
$$n=1,2. \quad (54)$$

This enables us to rewrite Eqs. (41) and (53) in the form

$$[\omega-6K]G_1(\mathbf{r}_j,\mathbf{r}_k,\omega)$$
$$=\delta_{\mathbf{r}_j,\mathbf{r}_k}-K\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',\mathbf{r}_k,\omega)+\rho U_0G_2(\mathbf{r}_j,\mathbf{r}_k,\omega), \quad (55)$$

$$[\omega-6K-\rho U_0]G_2(\mathbf{r}_j,\mathbf{r}_k,\omega)$$
$$=2\delta_{\mathbf{r}_j,\mathbf{r}_k}-2K\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',\mathbf{r}_k,\omega)$$
$$+K\sum_{\mathbf{r}'}\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle G_1(\mathbf{r}_j,\mathbf{r}_k,\omega). \quad (56)$$

If we denote by $G_1{}^0$ and $G_2{}^0$ the Green's functions in the absence of the off-diagonal elements of the kinetic energy, then these functions satisfy the equations

$$[\omega-6K]G_1{}^0(\mathbf{r}_j,\mathbf{r}_k,\omega)=\delta_{\mathbf{r}_j,\mathbf{r}_k}+\rho U_0G_2{}^0(\mathbf{r}_j,\mathbf{r}_k,\omega), \quad (57)$$

$$[\omega-6K-\rho U_0]G_2{}^0(\mathbf{r}_j,\mathbf{r}_k,\omega)=2\delta_{\mathbf{r}_j,\mathbf{r}_k}. \quad (58)$$

Solving for $G_1{}^0$ we get

$$G_1{}^0(\mathbf{r}_j,\mathbf{r}_k,\omega)=\delta_{\mathbf{r}_j,\mathbf{r}_k}A(\omega), \quad (59)$$

where

$$A(\omega)=\frac{-1}{\omega-6K-i\eta}+\frac{2}{\omega-6K-\rho U_0+i\eta}, \quad (60)$$

and where we have shifted the poles of $G_1{}^0$ off the real axis by the infinitesimal η. That this is the correct prescription is easily checked by calculating the time-dependent $G_1{}^0(\mathbf{r}_j,t;\mathbf{r}_k,t')$ which is, using Eq. (54),

$$G_1{}^0(\mathbf{r}_j,t;\mathbf{r}_k,t')$$
$$=\frac{\delta_{\mathbf{r}_j,\mathbf{r}_k}}{2\pi}\int_{-\infty}^{\infty}A(\omega)e^{-i\omega(t-t')}d\omega$$
$$=-i\delta_{\mathbf{r}_j,\mathbf{r}_k}\exp[-i6K(t-t')], \qquad t<t' \quad (61)$$
$$=-2i\delta_{\mathbf{r}_j,\mathbf{r}_k}\exp[-i(6K+\rho U_0)(t-t')], \quad t>t'.$$

These are the correct values for the completely localized state with one particle in each cell. For $t<t'$, $G_1{}^0$ represents hole propagation, while for $t>t'$ it represents propagation of an excess particle. The function $G_1{}^0$ satisfies the sum rule for a single-particle Green's function

$$i\lim_{t\to 0+}[G_1{}^0(\mathbf{r}_j,t;\mathbf{r}_k,0)-G_1{}^0(\mathbf{r}_j,-t;\mathbf{r}_k,0)]=\delta_{\mathbf{r}_j,\mathbf{r}_k}. \quad (62)$$

The constraint of N particles in our system is satisfied since, from Eq. (61), we have

$$\langle b_{\mathbf{r}_j}{}^{\dagger}b_{\mathbf{r}_j}\rangle=i\lim_{t'\to t+}G_1{}^0(\mathbf{r}_j,t;\mathbf{r}_j,t')=1. \quad (63)$$

The energy $6K+\rho U_0$ appearing in the exponential of Eq. (60) for $t>t'$ represents the energy to add one more particle to the ground state, whereas the energy $6K$ appearing in $G_1{}^0$ for $t<t'$ is the negative of the energy to remove one particle from the N particle ground state. Thus, we see that we have an energy gap, which reflects the asymmetry between particles and holes.[7] In this completely localized ground state, one would naturally expect the particle momentum distribution to be uniform over the range of admissible k values. This anticipated result follows by transforming $G_1{}^0$ to momentum space:

$$G_1{}^0(\mathbf{r}_j,\mathbf{r}_k,\omega)=[(2\pi)^3\rho]^{-1}\int G_1{}^0(\mathbf{k},\omega)e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_k)}d^3k, \quad (64)$$

where $-\pi/r_0\leq k_s\leq\pi/r_0$, $s=x,y,z$. We can determine $|\varphi^0(\mathbf{k})|^2$, the probability distribution for single-particle momenta, by introducing Eq. (64) into (53), and substituting the result into Eq. (63)

$$1=i[(2\pi)^4\rho]^{-1}\int\int G_1{}^0(\mathbf{k},\omega)e^{i\omega 0^+}d\omega d^3k. \quad (65)$$

Writing this in the form

$$1=[(2\pi)^3\rho]^{-1}\int|\varphi^0(\mathbf{k})|^2d^3k, \quad (66)$$

we identify $|\varphi^0(\mathbf{k})|^2$ as

$$|\varphi^0(\mathbf{k})|^2=i(2\pi)^{-1}\int G_1{}^0(\mathbf{k},\omega)e^{i\omega 0^+}d\omega. \quad (67)$$

For our localized state we get $G_1{}^0(\mathbf{k},\omega)$ from Eq. (58) as

$$G_1{}^0(\mathbf{k},\omega)=A(\omega), \quad (68)$$

whereupon

$$|\varphi^0(\mathbf{k})|^2=1, \quad (69)$$

for all $\mathbf{k}$'s in the range cited earlier.

[7] The chemical potential μ is not a pole of our one-particle Green's function. For the completely localized state here being considered, μ, the difference in energy between the ground state for $N\pm 1$ particles and the ground state for N particles (at constant volume), is equal to $10K$. There is no pole of G_1 corresponding to this energy difference because the cell creation and destruction operators have zero matrix elements between the states referred to.

Returning now to the general case in which the off-diagonal elements of the kinetic energy operator are present, we find solutions of $G_2(\mathbf{r}_j,\mathbf{r}_k,\omega)$ and $G_1(\mathbf{r}_j,\mathbf{r}_k,\omega)$ in the form

$$G_2(\mathbf{r}_j,\mathbf{r}_k,\omega)=f(\omega)[\delta_{\mathbf{r}_j,\mathbf{r}_k}-K\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',\mathbf{r}_k,\omega)+\tfrac{1}{2}hKG_1(\mathbf{r}_j,\mathbf{r}_k,\omega)], \quad (70)$$

where

$$f(\omega)=2/(\omega-6K-\rho U_0+i\eta), \quad h=\sum_{\mathbf{r}'}\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle, \quad (71)$$

$$G_1(\mathbf{r}_j,\mathbf{r}_k,\omega)=A(\omega)[\delta_{\mathbf{r}_j,\mathbf{r}_k}-K\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',\mathbf{r}_k,\omega)]+KhB(\omega)G_1(\mathbf{r}_j,\mathbf{r}_k,\omega), \quad (72)$$

where

$$B(\omega)=-1/(\omega-6K-i\eta)+1/(\omega-6K-\rho U_0+i\eta). \quad (73)$$

We now make a momentum resolution

$$(2\pi)^3G_m(\mathbf{r}_j,\mathbf{r}_k,\omega)=\int G_m(\mathbf{k},\omega)e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_k)}d^3k, \quad m=1,2, \quad (74)$$

in which the range of integration is identical to that previously indicated for Eq. (64). With this replacement made in Eq. (72), G_1 satisfies

$$[1+2KG_1{}^0(\mathbf{k},\omega)\sum_i\cos k_i\cdot r_0-KhB(\omega)]G_1(\mathbf{k},\omega)=G_1{}^0(\mathbf{k},\omega). \quad (75)$$

Using the value for $G_1{}^0$ given in Eq. (59), we find that G_1 can be written in a form which explicitly displays its singularities

$$G_1(\mathbf{k},\omega)=\frac{\omega-6K+\rho U_0}{\omega_+-\omega_-}\left[\frac{1}{\omega-\omega_+}-\frac{1}{\omega-\omega_-}\right], \quad (76)$$

where

$$\omega_\pm=6K+\tfrac{1}{2}\rho U_0-K\sum_i\cos k_i\cdot r_0 \pm\{(\tfrac{1}{2}\rho U_0-K\sum_i\cos k_i\cdot r_0)^2-2K\rho U_0\sum_i\cos k_i\cdot r_0+\rho U_0Kh\}^{1/2}\mp i\eta. \quad (77)$$

Since the singularities of G_1 depend through the parameter h on G_1 itself, the solution for G_1 in Eq. (76) is of a self-consistent form. For convenience we shift the energy by the amount $6K$, the kinetic energy for localization of a particle in a cell, that is

$$\epsilon=\omega-6K, \quad (78)$$

and we introduce the following ratio of kinetic energy of localization to potential energy:

$$x=2K/\rho U_0=\rho^{2/3}/m\rho U_0. \quad (79)$$

Then Eq. (77) becomes

$$\epsilon_\pm=\tfrac{1}{2}\rho U_0\{(1-x\sum_i\cos k_i\cdot r_0)\pm[(1-x\sum_i\cos k_i\cdot r_0)^2-4x\sum_i\cos k_i\cdot r_0+2hx]^{1/2}\}. \quad (80)$$

We may now obtain the values for the smallest energy differences between the ground state and the two states representing one particle added and one particle removed.

For small x, expansion of the square root in Eq. (80) yields the following result, correct to first power in x:

$$(\omega_+)_{\min}=6K+\rho U_0(1-6x), \quad (\omega_-)_{\max}=6K+3x\rho U_0. \quad (81)$$

We can interpret these results qualitatively in the following manner. The energy to add one particle to the N-particle state has decreased from its value ρU_0+6K found earlier for the completely localized state to $\rho U_0(1-6x)+6K$. This appears reasonable since now when we add a particle to a given cell, that cell may be vacant, costing no potential energy. Thus, in the context of the foregoing approximation, we can interpret $(1-6x)$ as the probability that a given cell is occupied by one particle. In the same way, the increase in ω_- from $6K$ to $6K+3x\rho U_0$ is due to the fact that now when we remove a particle from the N-particle ground state, it may come from a doubly occupied cell, in which event its removal releases ρU_0 units of energy. Hence, within the limits of our approximation, we can interpret $3x$ as the probability for a double occupancy of a given cell. It is noted that, as the density decreases, the parameter $x=\rho^{2/3}/m\rho U_0$ increases, assuming the effective interaction U_0 is constant.

For general values of x, the aforementioned energy differences are determined by the poles at $(\omega_+)_{\min}$ and $(\omega_-)_{\max}$, which occur, of course, for zero momentum. These are obtained from Eq. (80) as

$$\omega_\pm(k=0)=6K+\tfrac{1}{2}\rho U_0\{1-3x\pm[(1-3x)^2-12x+2hx]^{1/2}\}. \quad (82)$$

The energy gap is given by

$$\omega_+(k=0)-\omega_-(k=0)=\rho U_0[(1-3x)^2-12x+2hx]^{1/2}. \quad (83)$$

The excited states of one particle character for small momenta can be obtained from Eq. (80) in the form

$$\omega_\pm(k)\cong 6K+\tfrac{1}{2}\rho U_0\left\{1-3x+\frac{k^2}{2m\rho U_0}\pm\left[(1-3x)^2-12x+2hx+3(1-x)\frac{k^2}{m\rho U_0}+\left(\frac{k^2}{2m\rho U_0}\right)^2\right]^{1/2}\right\}. \quad (84)$$

Equation (84) shows that, so long as the constant term inside the square root does not vanish, the excited states display a quadratic dependence of energy on momentum.

To simplify the subsequent analysis, we will replace the parameter h by its first approximation. As shown

in Appendix B, this is given by

$$h=\sum_{r'}\langle b_{r_j+r'}{}^{\dagger}b_{r_j}\rangle\cong 12x. \tag{85}$$

As x increases, or as the density ρ decreases, the energy gap decreases, and finally disappears at the value $x=x_0\cong 0.06$, which satisfies the equation

$$(1-3x_0)^2-12x_0+24x_0^2=0. \tag{86}$$

The smallness of x_0 indicates the insensitivity of the critical density to the precise value of h. At the value x_0, the constant term inside the square root of Eq. (84) vanishes, with the consequence that the excited single-particle energy dependence on momenta changes to the form

$$\omega_{\pm}(k)\cong\tfrac{1}{2}\rho U_0(1+3x_0)+\frac{k^2}{4m} \pm\frac{1}{2}\left[\frac{k^2}{2m}\left(\frac{k^2}{2m}+6(1-x_0)\rho U_0\right)\right]^{1/2}. \tag{87}$$

For small momenta, $k\ll(m\rho U_0)^{1/2}$, we now have a linear dependence of ω on k, as Eq. (87) indicates. The last factor in this equation differs from the Bogoliubov phonon spectrum given by Eq. (32) only in the numerical coefficient of the interaction term ρU_0. We may also note that the result $\omega_{\pm}(0)=\frac{1}{2}\rho U_0(1+3x_0)$ is, apart from the presence of the term $(1+3x_0)$ instead of unity, the same as the energy per particle at low density as calculated in Eq. (25), where all particles were assumed to be in the state with zero momentum.

One would expect that the aforementioned change in the character of the excitation spectrum and the vanishing of the energy gap as x approaches x_0 should be accompanied by a rather drastic change in the momentum distribution of the particles in the ground state. This we can check using Eq. (76) for $G_1(\mathbf{k},\omega)$ and identifying the probability distribution for momenta in analogy with Eq. (67), namely,

$$|\varphi(\mathbf{k})|^2=ic(2\pi)^{-1}\int G_1(\mathbf{k},\omega)e^{i\omega 0^+}d\omega =c(\omega_--6K+\rho U_0)/(\omega_+-\omega_-), \tag{88}$$

where c is a normalizing factor. Near x_0, the denominator of Eq. (88) goes to zero linearly with k, and $|\varphi(\mathbf{k})|^2$ approaches infinity as k approaches zero. (The integrated probability distribution remains finite due to the k^2 weighting factor in the integrand.)

Further increase in the parameter x above x_0, or equivalent decrease in the density below the corresponding ρ_0 is not possible within the present approximation of limited fluctuations. As Eqs. (76) and (77) show, G_1 would then have poles off the real energy axis for momenta equal to and near zero, indicating instability of the approximation with respect to these excitations. For densities less than ρ_0, it is necessary to return to the original Green's function equations and make allowance for the large fluctuations in number density accompanying the greatly increased occupation of zero momentum states. We have not yet succeeded in unambiguously demonstrating that the new approximation yields the well-known results for the boson gas at low densities.

IV. SUMMARY

At high densities, the ground state for bosons with repulsive interactions is represented by a wave function which localizes particles in small spatial regions. This implies a uniform distribution of single-particle momenta. The effect of the kinetic energy, regarded as a perturbation, is to cause virtual transitions which spread out the state over larger spatial regions, implying increased occupation of the small momentum levels. With decreasing density, the spread out region increases spatially, until finally, at a critical density, all localized character is essentially lost. At this density, the asymmetry between particles and holes disappears, and the dependence on small momenta of the energy for a single-particle excitation changes from quadratic to linear.

APPENDIX A

We present here the mathematical manipulations by means of which the transformation of Eq. (27),

$$b_{r_j}=1+\xi_{r_j},$$

converts the cell model Hamiltonian given by Eq. (16),

$$H=6K\sum_{r_j}b_{r_j}{}^{\dagger}b_{r_j}-K\sum_{r_j,r'}b_{r_j}{}^{\dagger}b_{r_j+r'} +\tfrac{1}{2}\rho U_0\sum_{r_j}b_{r_j}{}^{\dagger}b_{r_j}{}^{\dagger}b_{r_j}b_{r_j},$$

into the Hamiltonian of Eq. (28),

$$H=\tfrac{1}{2}N\rho U_0+K\sum_{r_j}(6\xi_{r_j}{}^{\dagger}\xi_{r_j}-\sum_{r'}\xi_{r_j}{}^{\dagger}\xi_{r_j+r'}) +\tfrac{1}{2}\rho U_0\sum_{r_j}(\xi_{r_j}{}^{\dagger}\xi_{r_j}{}^{\dagger}+2\xi_{r_j}{}^{\dagger}\xi_{r_j}+\xi_{r_j}\xi_{r_j}),$$

which yields the phonon spectrum.

Introducing Eq. (27) into Eq. (16) and considering the ξ's to be sufficiently small compared to unity such that products of three or more can be neglected, one obtains the result

$$\begin{aligned}H=&\tfrac{1}{2}N\rho U_0+K\sum_{r_j}(6\xi_{r_j}{}^{\dagger}\xi_{r_j}-\sum_{r'}\xi_{r_j}{}^{\dagger}\xi_{r_j+r'})\\ &+\tfrac{1}{2}\rho U_0\sum_{r_j}(\xi_{r_j}{}^{\dagger}\xi_{r_j}{}^{\dagger}+2\xi_{r_j}{}^{\dagger}\xi_{r_j}+\xi_{r_j}\xi_{r_j})\\ &+K\sum_{r_j}(6\xi_{r_j}-\sum_{r'}\xi_{r_j+r'})\\ &+\rho U_0\sum_{r_j}(\xi_{r_j}{}^{\dagger}+\xi_{r_j}+\xi_{r_j}{}^{\dagger}\xi_{r_j}).\end{aligned} \tag{A1}$$

The last term above is zero, as evidenced by application of the inverse transformation to this term:

$$\sum_{r_j}(\xi_{r_j}{}^{\dagger}+\xi_{r_j}+\xi_{r_j}{}^{\dagger}\xi_{r_j})=\sum_{r_j}(b_{r_j}{}^{\dagger}b_{r_j}-1)=\sum_{r_j}b_{r_j}{}^{\dagger}b_{r_j}-N=0.$$

Equation (A1) now reduces to Eq. (28) with the exception of the second last term,

$$K\sum_{r_j}(6\xi_{r_j}-\sum_{r'}\xi_{r_j+r'}). \tag{A2}$$

We can now show that this term is zero by noting that under the transformation to plane wave operators,

$$\xi_{\mathbf{r}_j}=N^{-1/2}\sum_{\mathbf{k}} a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}_j},$$

Eq. (A2) becomes

$$\begin{aligned}K\sum_{\mathbf{r}_j}(6\xi_{\mathbf{r}_j}-\textstyle\sum_{\mathbf{r}'}\xi_{\mathbf{r}_j+\mathbf{r}'})&=KN^{-1/2}\textstyle\sum_{\mathbf{r}_j}\sum_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}_j}(6-\sum_{\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{r}'})\\&=KN^{1/2}\textstyle\sum_{\mathbf{k}}a_{\mathbf{k}}\delta_{\mathbf{k},0}(6-\sum_{\mathbf{r}'}e^{i\mathbf{k}\cdot\mathbf{r}'})\\&=0.\end{aligned}$$

APPENDIX B

In this Appendix, we calculate the first approximation to the parameter h given in Eq. (85)

$$h=\textstyle\sum_{\mathbf{r}'}\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle\cong 12x.$$

We start from the definition of $G_1(\mathbf{r}_j,\mathbf{r}_k,\omega)$ in Eq. (54) from which there follows the relation

$$\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle=\frac{i}{2\pi}\int G_1(\mathbf{r}_j+\mathbf{r}',\,\mathbf{r}_j,\,\omega)e^{i\omega 0^+}d\omega. \tag{B1}$$

The function $G_1(\mathbf{r}_j,\mathbf{r}_k,\omega)$ is a solution of Eq. (72) which reads

$$\begin{aligned}G_1(\mathbf{r}_j,\mathbf{r}_k,\omega)=A(\omega)[\delta_{\mathbf{r}_j,\mathbf{r}_k}-K\textstyle\sum_{\mathbf{r}'}G_1(\mathbf{r}_j+\mathbf{r}',\,\mathbf{r}_k,\,\omega)]\\+KhB(\omega)G_1(\mathbf{r}_j,\mathbf{r}_k,\omega),\end{aligned} \tag{B2}$$

where

$$A(\omega)=\frac{-1}{\omega-6K-i\eta}+\frac{2}{\omega-6K-\rho U_0+i\eta},$$

$$B(\omega)=\frac{-1}{\omega-6K-i\eta}+\frac{1}{\omega-6K-\rho U_0+i\eta}.$$

We develop a series solution in powers of the kinetic energy K:

$$\begin{aligned}G_1(\mathbf{r}_j,\mathbf{r}_k,\omega)&=\sum_{n=0}^{\infty}K^nG_1{}^{(n)}(\mathbf{r}_j,\mathbf{r}_k,\omega),\\\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle&=\sum_{n=1}^{\infty}K^n\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle^{(n)}.\end{aligned} \tag{B3}$$

With these substitutions in Eq. (B2), we obtain

$$\begin{aligned}G_1{}^{(0)}(\mathbf{r}_j,\mathbf{r}_k,\omega)&=A(\omega)\delta_{\mathbf{r}_j,\mathbf{r}_k},\\G_1{}^{(1)}(\mathbf{r}_j,\mathbf{r}_k,\omega)&=-A^2(\omega)\textstyle\sum_{\mathbf{r}''}\delta_{\mathbf{r}_j+\mathbf{r}'',\mathbf{r}_k},\\G_1{}^{(2)}(\mathbf{r}_j,\mathbf{r}_k,\omega)&=A^3(\omega)\textstyle\sum_{\mathbf{r}'',\mathbf{r}'}\delta_{\mathbf{r}_j+\mathbf{r}''+\mathbf{r}',\mathbf{r}_k}\\&\quad+B(\omega)A(\omega)\textstyle\sum_{\mathbf{r}'}\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle^{(1)}\delta_{\mathbf{r}_j,\mathbf{r}_k}.\end{aligned} \tag{B4}$$

Then the first approximation yields

$$\begin{aligned}\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle^{(1)}&=\frac{iK}{2\pi}\int G_1{}^{(1)}(\mathbf{r}_j+\mathbf{r}',\,\mathbf{r}_j,\,\omega)e^{i\omega 0^+}d\omega\\&=-\frac{iK}{2\pi}\sum_{\mathbf{r}''}\delta_{\mathbf{r}_j+\mathbf{r}'+\mathbf{r}'',\mathbf{r}_j}\int A^2(\omega)e^{i\omega 0^+}d\omega\\&=-(iK/2\pi)(8\pi i/\rho U_0)=4K/\rho U_0=2x.\end{aligned} \tag{B5}$$

Consequently,

$$\textstyle\sum_{\mathbf{r}'}\langle b_{\mathbf{r}_j+\mathbf{r}'}{}^{\dagger}b_{\mathbf{r}_j}\rangle^{(1)}=12x, \tag{B6}$$

which is Eq. (85).

This series solution for G_1 can be utilized to evaluate the ground-state energy in powers of the parameter x. The results obtained in this way agree with a Rayleigh-Schrödinger perturbation treatment which was previously carried out,[8] and which proved to be analogous to a sequence of restricted random walk problems.

[8] G. C. Knollman, Ph.D. thesis, Georgia Institute of Technology, 1961 (unpublished).