

where

$$I(k, \alpha) = \int_{-\infty}^{\infty} du \frac{F_i(u)}{|\epsilon^-(u)|^2} \quad (\text{D25})$$

and $\alpha \equiv \theta_e/\theta_i$.

Observe that in the limit of large k , $I(k, \alpha) \rightarrow 1$, $\rho(0) \rightarrow 1$, $\epsilon^-(-w) \rightarrow 1$, and Eq. (D24) becomes identical to Eq. (D20). Consequently, the dominant contribution from σ_{13} , for all k , is just the first term in Eq. (D24). Adding this expression to the first term in Eq. (D7) we obtain the final result

$$\sigma_1(\omega) = iA \int dk \frac{F_e^-(w)}{\epsilon^-(-w)\epsilon(0)} G(k, \alpha), \quad (\text{D26})$$

where

$$G(k, \alpha) = 1 - \left(1 - \frac{1}{\alpha}\right) \left(1 + \frac{k_d^2}{k^2}\right) \left(1 + \frac{k_e^2}{k^2}\right) I(k, \alpha). \quad (\text{D27})$$

This result is identical to Eqs. (30) and (31).

Effect of Attractive Forces on the Solid-Superfluid Transition in He⁴ at Absolute Zero*

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The effect of attractive interactions between helium atoms on the solid-superfluid transition in He⁴ at absolute zero is considered. It is found that the density of the solid-superfluid transition does not depend on the strength of the attractive interactions, but only on the mass of the particles and the strength of the repulsive interactions. The density at which the system reaches zero pressure increases with increasing strength of attractive forces, so that sufficiently large attractive forces can inhibit the transition. Quantitative estimates and comparisons are made of the zero-pressure density and of the transition density, for different masses and for different strengths of attractive interactions.

I. INTRODUCTION

THIS paper describes the effect of attractive interactions on the zero-temperature transition from a solid to a superfluid state, utilizing a cell model.¹ In a previous work, it was demonstrated that such a transition occurs when the attractive interactions between particles are assumed to play no role in the dynamics of the system.² Here we try to assess the importance of these attractive forces outside the repulsive core in inhibiting the solid-superfluid transition. We find that the attractive forces do not affect the density of the transition, a circumstance due mainly to (a) the small size of the attractive intercell interactions compared with the repulsive intracell interactions, which is necessary for stability of the solid lattice, and (b) the more

important role played by the off-diagonal kinetic energy (overlap) terms. The attractive forces do influence the macroscopic behavior of the system through their effect on the pressure. The stronger the attractive forces, the larger the density at which the pressure goes to zero. Sufficiently large attractive forces cause the zero-pressure density to be larger than the transition density, so that the solid would have to be placed under negative pressure in order to reach the solid-superfluid transition density.

In Sec. II, we describe the qualitative features of the cell model and of the dependence of the kinetic and potential energy terms in the Hamiltonian on the degree of density fluctuations. Section III shows how a truncation of the Green's-function equations yields results equivalent to our earlier treatment. In an Appendix, we outline the proof that an improved truncation of the Green's-function equations still results in a negligible effect of attractive interactions on the dynamics. Finally, in Sec. IV we compare the density at zero pressure with the density at the solid-superfluid transition, for Bose systems having different strengths of the

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¹ H. A. Gersch and G. C. Knollman, Phys. Rev. **129**, 959 (1963).

² H. A. Gersch and J. M. Tanner, Phys. Rev. **139**, A1769 (1965).

attractive forces and different masses. This comparison shows that we should not expect the solid-superfluid transition for the Bose system composed of the lighter mass atoms of hydrogen in solid H₂, where the effects of the lighter mass are outweighed by the greatly increased interactions.

A word of caution should be given about the limitations of our equations. In this paper the excitations $\epsilon(k)$ in the solid phase are quadratic in the momentum k . We believe this feature is due to our approximations on the Green's-function equations and do not represent a characteristic of the cell model. One reason for this belief is that one can find, in this cell model, the equations of motion of the Green's function for the density fluctuations, $\langle T\rho_k(t)\rho_k^\dagger(0) \rangle$ where $\rho_k = \sum_j b_j^\dagger b_j e^{-ikj}$ is the k th Fourier coefficient of the density fluctuations. Then utilizing the random phase approximation, one gets the usual equations that yield sound-wave excitations, $\epsilon(k) \sim ck$ for low k both in the solid and fluid phases. Now to get the correct excitation spectrum linear in k for low k , one must always have zero-point collective motions in the ground state to start with. This implies that we have by our approximations removed such ground-state collective behavior. Zero-point collective motion contributes to the ground-state energy E_0 with a term proportional to $m^{-1/2}$, where m is the particle mass. We have no such term in our results. It was shown by London³ that the zero-point energy is proportion to m^{-1} for He⁴, H₂, HD, and D₂. That is, the zero-point collective behavior, although necessary to obtain the correct excitation spectrum, contributes negligibly to the ground-state energy of the system. The important contribution is due to the localization energy of the particles. This represents another case where the wave function is very sensitive to the approximations while the ground-state energy E_0 is rather insensitive.

The results of Gersch and Knollman¹ and Gersch and Tanner² can be interpreted to mean that the macroscopic occupation of the zero-momentum level (off-diagonal long-range order) occurring at a critical density, as one lowers the density of solid He⁴ at $T=0$, is rather insensitive to the approximations performed.

Our analysis in this work is based on arguments centered on macroscopic parameters such as energy, pressure, and the onset of macroscopic occupation of the zero momentum level, but not on the details of the wave function or the excitation spectrum of the system.

II. THE CELL MODEL

The space occupied by the system under consideration is divided into cubic cells of volume equal to the molecular specific volume. In this model one considers the state of the system to be specified completely if one knows the probability amplitude for finding n_j particles in the j th cell, for $n_j = 1, 2, \dots, N$ and $j = 1, 2, \dots, N$, where N

is the total number of particles in the system. That is to say, one considers the particle motions from cell to cell but not the motion within a cell. This is equivalent to the formal statement

$$\psi(r) = \sum_{j=1}^N b_{rj} \delta_{r,rj} \rho^{1/2}, \quad (1)$$

where $\psi(r)$ is the usual destruction operator for a particle at the point r , $\rho = N/V$ is the particle density, and $\delta_{r,rj}$ is a Kronecker delta function. For bosons, we have the commutation relation

$$[\psi(r), \psi^\dagger(r')] = \delta(r-r'), \quad (2)$$

which along with Eq. (1) implies the commutation relations

$$[b_{rj}, b_{rk}^\dagger] = \delta_{rj, rk}, \quad [b_{rj}, b_{rk}] = [b_{rj}^\dagger, b_{rk}^\dagger] = 0. \quad (3)$$

The operator b_{rj} destroys a particle in the j th cell, and $b_{rj}^\dagger$ creates one. For a more detailed description of the model see Refs. 1 and 2. From the usual expression for the Hamiltonian of a system of bosons with two-body interactions⁴ and Eq. (1), one arrives at the following expression

$$H = 6K \sum_j b_j^\dagger b_j - K \sum_{j,\delta} b_j^\dagger b_{j+\delta} + \frac{\rho U_0}{2} \sum_j b_j^\dagger b_j^\dagger b_j b_j + \frac{\rho V}{2} \sum_{j,\delta} b_j^\dagger b_j b_{j+\delta}^\dagger b_{j+\delta}, \quad (4)$$

where the notation has been simplified by replacing the lattice vector $\mathbf{r}_j$ by its index j .

The sum on δ in the second term on the right-hand side of Eq. (4) is over the nearest neighbors, and in the last term as well if one limits the range of the interaction to nearest neighbors. This nearest-neighbor approximation is used to simplify the notation in the subsequent discussion, although in the actual application of intercell interactions, we employ a lattice sum over all neighbors of the Yntema Schneider potential given by Eq. (73). In Eq. (4) $K = (\hbar^2 \rho^{2/3})/2m$ is the kinetic energy of localization, where $\rho = N/V$ is the particle density,

$$U_0 = \int U(r) d\tau, \quad r \text{ in one cell}, \quad (5)$$

measures the repulsive interaction between a pair of particles in a cell, and

$$V = \rho \int U(r-r') d\tau d\tau', \quad \begin{aligned} r &\text{ in cell } j, \\ r' &\text{ in cell } j+\delta. \end{aligned} \quad (6)$$

Here $U(r-r')$ is the two-body interaction potential. These forms for K and V are intended to have only

³ F. London, *Superfluids* (Dover Publications, Inc., New York, 1964), Vol. II, p. 34.

⁴ A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963), Chap. 1.

Configuration	Probability a)	Amplitudes b)
	$e^{1/2}$	$e^{1/2}$
	z	z
	y	z
	h	z^2
	τ	z^2

FIG. 1. Probability amplitudes for possible local configurations in the ground state of the cell model assuming, (a) correlations between the density fluctuations, (b) no correlations.

qualitative significance; in Sec. IV we introduce more realistic expressions for them.

In Ref. 1 there was obtained an instability in the description of the ground state for the Boson system for densities ρ below a critical value ρ_0 . The instability was associated with a solid superfluid transition in Ref. 2. In these works, no account of the effect of attractive nearest-neighbor interactions on the dynamics of the system was taken. The main purpose of the present work is to consider the effect of such interactions represented by the last term in the Hamiltonian in Eq. (4). It is important to do so since the strength of the attractive interaction is one of the two quantities that make the difference between superfluid He^4 at absolute zero and solid hydrogen or neon, for example.

Before proceeding any further it is important to note that $|V| \ll U_0$. This can be shown by a simple argument in which we consider, at extremely high densities, the energies of two possible configurations. Let the first configuration correspond to one particle per cell. The energy of this system is $(6K + 3\rho V)N$. Now consider a system with half its volume occupied by particles and the other half empty, with $n_j = 2$ for $j = 1, 2, \dots, N/2$ and $n_j = 0$ for $j = N/2 + 1, \dots, N$. The energy associated with this system is $(6K + \rho U_0/2 + 6\rho V)N$. Now $V < 0$, so in order to have the first configuration favored over the second one for the ground state of the system at extremely high densities we must have

$$U_0/6 > |V|. \quad (7)$$

We will be concerned in this paper with the behavior of a system of bosons in the ground state. To illustrate some features of the cell model we will now give a brief argument to obtain a rough value of the fluctuations $\langle n_j^2 - n_j \rangle$ as a function of density, for the ground state $|\phi_0\rangle$. Let us focus attention on the j th cell and its six nearest neighbors (we assume a simple cubic lattice), and let z be the probability amplitude for finding zero or two particles in a cell, with zero probability for finding more than two particles in a cell. The probability for finding one particle in a cell is then equal to $1 - 2z^2$. In Fig. 1 we show some local configurations and assign them probability amplitudes under the two circum-

stances, (a) that there exist correlations between the density fluctuations, and (b) assuming no correlations. Since z is assumed to be small, other possible configurations corresponding to high-density fluctuations would give negligible contributions to the ground state. It is reasonable to assign relative orders of magnitude to the probability amplitudes labeled in Fig. 1,

$$y < z, \quad h \ll z, \quad \tau \leq z.$$

If there were no correlations we would obtain

$$\langle \sum_{j,\delta} b_j^\dagger b_{j+\delta} \rangle \approx z^2 + \text{negligible terms.}$$

However, with correlations, we obtain

$$\langle \sum_{j,\delta} b_j^\dagger b_{j+\delta} \rangle \approx z + \text{negligible terms.} \quad (8)$$

With regard to the last term in the Hamiltonian, Eq. (4), it will suffice for the moment to say that it has a minimum expectation value for $z = 0$. Therefore if there are going to be any fluctuations in the system in the ground state which minimizes $\langle H \rangle$ it is necessary that

$$\langle K \sum_{j,\delta} b_j^\dagger b_{j+\delta} \rangle \gtrsim (\rho U_0/2) \langle \sum_j b_j^\dagger b_j^\dagger b_j b_j \rangle,$$

for z approaching zero, since both these terms are zero when z is zero. Now

$$\langle n_j^2 - n_j \rangle = \langle b_j^\dagger b_j^\dagger b_j b_j \rangle \sim z^2, \quad (9)$$

so if we assume no correlations, requiring the energy to be minimum implies a value for z determined by

$$Kz^2 \gtrsim (\rho U_0/2)z^2.$$

However, for high densities, $(\rho U_0/2K) \gg 1$, so that the condition can only be met with $z = 0$, i.e., no correlations imply no fluctuations. If on the other hand we assume correlations, then minimum energy implies

$$K\tau \gtrsim (\rho U_0/2)z^2. \quad (10)$$

However, as we previously mentioned,

$$\tau \leq z. \quad (11)$$

Therefore

$$2K/\rho U_0 \gtrsim z. \quad (12)$$

Using the value for K previously given, we have

$$z \lesssim (\hbar^2/mU_0\rho^{1/3}). \quad (13)$$

We see that the fluctuations in the ground state decrease as the density increases as was to be expected. Our approximations in this work will be such that they become asymptotically exact as $z \rightarrow 0$, i.e., as $\rho \rightarrow \infty$. A little thought allows one to write

$$\begin{aligned} \langle z = 0 | \sum_{j,\delta} b_j^\dagger b_j b_{j+\delta}^\dagger b_{j+\delta} | z = 0 \rangle \\ - \langle z \neq 0 | \sum_{j,\delta} b_j^\dagger b_j b_{j+\delta}^\dagger b_{j+\delta} | z \neq 0 \rangle \lesssim Nz^2. \end{aligned} \quad (14)$$

It follows then from Eqs. (7)–(11) that the attractive-interaction term is of very small importance in minimiz-

ing $\langle H \rangle$. It should not be surprising, therefore, to find later that the attractive interaction term plays a very small role in the dynamics of the ground state of the system under consideration. The difference in behavior between He⁴ and H₂ or Ne²⁰ at $T=0$ will be found in the thermodynamics of the systems. We will return to these ideas later.

III. SOLUTION OF THE GREEN'S-FUNCTION EQUATIONS; INSTABILITY

We will attempt to describe the system of Bose particles defined by the Hamiltonian of Eq. (4) as the pressure decreases from a very high value to zero. The density ρ will then decrease from a correspondingly high value to the value $\rho(P=0)=\rho_1$ at which

$$\left\{ \frac{\partial}{\partial \rho} \langle \phi_0 | H(\rho) | \phi_0 \rangle \right\}_{\rho_1} = 0,$$

where $|\phi_0\rangle$ is the density-dependent ground-state vector function for the system. The value of ρ_1 at which the pressure is zero will depend on V , the strength of the attractive interactions. The density of the solid-fluid transition ρ_0 , if there is one, will be obtained. If $\rho_0 > \rho_1$, the system undergoes a transition, otherwise it does not.

The one-particle Green's function furnishes, as is well known, the energy spectrum of a system. It is of interest here to find out how the energy spectrum changes with the density of the system when the attractive interaction in Eq. (4) is included. In this way a density of transition will be obtained as well as the energy spectrum at the transition density. For this purpose we utilize the Green's functions introduced in Ref. 2 and defined by

$$G_j(l, t) = -i \langle T F_{lj}(t) b_l(t) b_0^\dagger(0) \rangle, \quad (15)$$

where $j=1, 2, 3$, and the operator $F_{lj}(t)$ is given by

$$[b_l^\dagger(t)]^{j-1} [b_l(t)]^{j-1}. \quad (16)$$

The symbol T in Eq. (15) is the time-ordering operator such that

$$T F_{lj}(t) b_l(t) b_0^\dagger(0) = \theta(t) F_{lj}(t) b_l(t) b_0^\dagger(0) + \theta(-t) b_0^\dagger(0) F_{lj}(t) b_l(t), \quad (17)$$

with

$$\begin{aligned} \theta(t) &= 1, \quad t > 0; \\ &= 0, \quad t < 0. \end{aligned} \quad (18)$$

Since

$$F_{lj}(t) b_l(t) = n_l(n_l-1) \cdots (n_l-j+2) b_l(t), \quad (19)$$

$G_j(l, t)$ describes particle ($t > 0$) or hole ($t < 0$) propagation weighted by the particle-fluctuation term $F_{lj}(t)$. By differentiating $G_j(l, t)$ with respect to time it is easily demonstrated that

$$\begin{aligned} [i\partial/\partial t - 6K - (j-1)\rho U_0] G_j(l, t) &= j\Delta_j \delta(t) \delta_{l,0} - jK D_j(l, t) \\ &+ (j-1)K E_j(l, t) + \rho U_0 G_{j+1}(l, t) - \rho V H_{j+1}(l, t), \end{aligned} \quad (20)$$

where

$$D_j(l, t) = -i \langle T F_{lj}(t) \sum_\delta b_{l+\delta}(t) b_0^\dagger(0) \rangle, \quad (21)$$

$$E_j(l, t) = -i \langle T \sum_\delta b_{l+\delta}^\dagger(t) F_{l, j-1}(t) b_l(t) b_l(t) b_0^\dagger(0) \rangle, \quad (22)$$

$$H_j(l, t) = -i \langle T \sum_\delta b_{l+\delta}^\dagger(t) b_{l+\delta}(t) F_{l, j-1}(t) b_l(t) b_0^\dagger(0) \rangle \quad (23)$$

$$\begin{aligned} \Delta_j &= 1, \quad j=1; \\ &= \langle n(n-1) \cdots (n-j+2) \rangle, \quad j \geq 2. \end{aligned} \quad (24)$$

The attractive interactions enter in the last term on the right-hand side of Eq. (20).

The first two equations in exact form are

$$\begin{aligned} [i(\partial/\partial t) - 6K] G_1(l, t) &= \delta(t) \delta_{l,0} - K D_1(l, t) \\ &+ \rho U_0 G_2(l, t) - \rho V H_2(l, t), \end{aligned} \quad (25)$$

$$\begin{aligned} [i(\partial/\partial t) - 6K - \rho U_0] G_2(l, t) &= 2\langle n \rangle \delta(t) \delta_{l,0} \\ &- 2K D_2(l, t) + K E_2(l, t) + \rho U_0 G_3(l, t) - \rho V H_3(l, t). \end{aligned} \quad (26)$$

The terms on the right-hand side of Eq. (26) may be approximated consistent with the concept of small fluctuations away from the localized high-density state. This approximation will result in Eqs. (25) and (26) forming a closed set of coupled equations. For the strictly localized system $|n_j=1\rangle$, which is the ground state in the high-density limit,

$$b_l^\dagger(t) b_l(t) |N, 0\rangle \rightarrow |N, 0\rangle. \quad (27)$$

Therefore as the density increases and the system approaches the localized state, we can make the following approximations previously introduced in Ref. 2:

$$\begin{aligned} D_2(l, t) &= -i \langle T b_l^\dagger(t) b_l(t) \sum_\delta b_{l+\delta}(t) b_0^\dagger(0) \rangle \rightarrow \\ &-i \sum_\delta \langle T b_{l+\delta}(t) b_0^\dagger(0) \rangle \\ &= \sum_\delta G_1(l+\delta, t), \end{aligned} \quad (28)$$

$$\begin{aligned} E_2(l, t) &= -i \langle T \sum_\delta b_{l+\delta}^\dagger(t) b_l(t) b_l(t) b_0^\dagger(0) \rangle \\ &\approx -i \sum_\delta \langle b_{l+\delta}^\dagger b_l \rangle \langle T b_l(t) b_0^\dagger(0) \rangle \\ &\approx g G_1(l, t), \end{aligned} \quad (29)$$

in which g is some as yet unspecified function of particle density. Also

$$\begin{aligned} G_3(l, t) &= -i \langle T b_l^\dagger(t) b_l^\dagger(t) b_l(t) b_l(t) b_0^\dagger(0) \rangle \\ &\approx -i \langle b_l^\dagger b_l^\dagger b_l b_l \rangle \langle T b_l(t) b_0^\dagger(0) \rangle \\ &\approx \chi G_1(l, t), \end{aligned} \quad (30)$$

where χ is another function of the particle density. The two functions g and χ will be shortly determined from a particle-conservation requirement. In addition to these approximations, we have to deal with the functions H_2 and H_3 which represent the attractive interactions. These we approximate in the spirit of limited fluctuations as

$$\begin{aligned} H_2(l, t) &= -i \langle T \sum_\delta b_{l+\delta}^\dagger(t) b_{l+\delta}(t) b_l(t) b_0^\dagger(0) \rangle \\ &\approx -i \sum_\delta \langle b_{l+\delta}^\dagger b_{l+\delta} \rangle \langle T b_l(t) b_0^\dagger(0) \rangle \\ &\approx 6G_1(l, t), \end{aligned} \quad (31)$$

and

$$\begin{aligned} H_3(l, t) &= -i \langle T \sum_{\delta} b_{l+\delta}^\dagger(t) b_{l+\delta}(t) b_l^\dagger(t) b_l(t) b_0^\dagger(0) \rangle \\ &\approx -i \sum_{\delta} \langle b_{l+\delta}^\dagger b_{l+\delta} \rangle \langle T b_l^\dagger(t) b_l(t) b_0^\dagger(0) \rangle, \quad (32) \\ &\approx 6G_2(l, t). \end{aligned}$$

With these approximations, our equations of motion for G_1 and G_2 become

$$\begin{aligned} (i(\partial/\partial t) - 6K - 6\rho V)G_1(l, t) \\ = \delta(t)\delta_{l,0} - K \sum_{\delta} G_1(l+\delta, t) + \rho U_0 G_2(l, t), \quad (33) \end{aligned}$$

$$\begin{aligned} (i(\partial/\partial t) - 6K - 6\rho V - \rho U_0)G_2(l, t) \\ = 2\delta(t)\delta_{l,0} - 2K \sum_{\delta} G_1(l+\delta, t) \\ + (Kg + \chi\rho U_0)G_1(l, t). \quad (34) \end{aligned}$$

If now we define the sum of the diagonal zero-point energy and lattice potential energy,

$$6K + 6\rho V = I_0, \quad (35)$$

then Eqs. (33) and (34) become identical to Eqs. (55) and (56) in Ref. 2, except for the delta-function singularities which were there incorporated into the boundary conditions. These previously obtained Green's-function equations evolved from a simpler Hamiltonian, obtainable from the complete Hamiltonian of Eq. (4) by replacing the attractive interaction term as follows:

$$(\rho V/2) \sum_{j,\delta} b_j^\dagger b_{j+\delta}^\dagger b_{j+\delta} b_j \rightarrow 3\rho V \sum_j b_j^\dagger b_j. \quad (36)$$

This means that our present approximation on the Green's-function equations expressed in Eqs. (33) and (34) have exactly the same effect as approximating the attractive term as expressed in Eq. (36). However, the approximation term in Eq. (36) plays no role in the dynamics of the system; it is just a constant term independent of density fluctuations, so that our approximations have done away with the dynamic role the attractive interactions might play. This effect persists in the improved approximation described below, and leads to our main conclusion that the attractive forces play only a minor role in the dynamics of the solid-superfluid transition.

Since our equations for G_1 and G_2 reduce to those previously obtained, which exhibit a solid-superfluid transition, we have again the possibility for such a transition. The transition comes about in the following way: The solutions for the Fourier transforms $G_1(k, t)$ and $G_2(k, t)$ are

$$iG_1(k, t) = a_1^+(k)\theta(t)e^{-i\nu^+ \rho U_0 t} + a_1^-(k)\theta(-t)e^{i\nu^- \rho U_0 t} \quad (37)$$

and

$$iG_2(k, t) = a_2^+(k)\theta(t)e^{-i\nu^+ \rho U_0 t} + a_2^-(k)\theta(-t)e^{-i\nu^- \rho U_0 t}, \quad (38)$$

with

$$a_1^\pm(k) = \frac{1}{2} \left[\frac{3 - xs(k)}{\nu^+(k) - \nu^-(k)} \pm 1 \right], \quad (39)$$

$$a_2^\pm(k) = \frac{1}{2} \left[\frac{1 - xs(k) + \gamma}{\nu^+(k) - \nu^-(k)} \pm 1 \right],$$

where

$$x = 2K/\rho U_0, \quad (40)$$

$$s(k) = \frac{1}{2} \sum_{\delta} e^{ik\delta}, \quad (41)$$

$$\gamma(x) = \frac{1}{2} xg(x) + \chi(x), \quad (42)$$

$$\nu^\pm(k) = \lambda + \frac{1}{2} [1 - xs \pm (1 - 6xs + x^2 s^2 + 4\gamma)^{1/2}], \quad (43)$$

$$\lambda = I_0/\rho U_0, \quad (44)$$

$$G_j(k, t) = \sum_l G_j(l, t) e^{-ikl}. \quad (45)$$

The parameter γ which contains the two unspecified functions g and χ which entered into our approximate truncation procedure is now fixed from the requirement that the average number of particles per cell is exactly equal to unity;

$$\begin{aligned} \langle n_0 \rangle &= \langle b_0^\dagger b_0 \rangle = -iG_1(l=0, t=0^-) \\ &= 1 = \frac{1}{2N} \sum_k \left\{ \frac{3 - xs(k)}{[1 - 6xs(k) + x^2 s^2 + 4\gamma]^{1/2}} - 1 \right\}. \quad (46) \end{aligned}$$

Replacing the sum by an integral results in the equation

$$3 = \frac{1}{\pi^3} \int_R [3 - xs(\theta)] f[x, s(\theta)] d^3\theta, \quad (47)$$

where R denotes the region $0 \leq \theta_1, \theta_2, \theta_3 \leq \pi$,

$$s(\theta) = \sum_{i=1}^3 \cos \theta_i, \quad (48)$$

and

$$f(x, s) = [1 - 6xs + x^2 s^2 + 4\gamma]^{-1/2}. \quad (49)$$

Equation (47) then determines γ as a function of x , and hence as a function of density. The function γ increases with decreasing density until that density for which

$$1 - 18x_0 + 9x_0^2 + 4\gamma(x_0) = 0 \quad (50)$$

with solution $x_0 \simeq 0.067$.² At this density the quantity $\nu_+(0) - \nu_-(0)$ appearing in the denominator in Eq. (39) is equal to zero. For smaller densities, the Green's-function solutions were shown to be given by

$$\begin{aligned} iG_1(k, t) &= \frac{\theta(t)}{2} \left(\frac{3 - xs}{f^{-1} + \eta} + 1 \right) e^{-i\omega^+ t} \\ &+ \frac{\theta(-t)}{2} \left(\frac{3 - xs}{f^{-1} + \eta} - 1 \right) e^{-i\omega^- t}, \quad (51) \end{aligned}$$

$$iG_2(k, t) = \frac{\theta(t)}{2} \left(\frac{1 - xs + \gamma_0}{f^{-1} + \eta} + 1 \right) e^{-i\omega^+ t} + \frac{\theta(-t)}{2} \left(\frac{1 - xs + \gamma_0}{f^{-1} + \eta} - 1 \right) e^{-i\omega^- t}, \quad (52)$$

where

$$f^{-1} = f^{-1}(x, s) = [6x(3-s) - x^2(9-s^2)]^{1/2}, \quad (53)$$

and $1/\eta$ is proportional to the zero-momentum occupation

$$\langle N_0 \rangle = \langle a_0^\dagger a_0 \rangle = \frac{1}{2} [3(1-x)/\eta - 1]. \quad (54)$$

The energy for the elementary excitations is $\epsilon(k)$, and in the liquid region, these are obtained from the relation

$$\omega^\pm(k) = \nu^\pm \rho U_0 = |E(N \pm 1, k) - E(N, 0)| = \mu \pm \epsilon(k). \quad (55)$$

From Eq. (43) there follows, for $\epsilon(k)$,

$$\epsilon(k) = K(3-s) + (\rho U_0/2) [6x(3-s)]^{1/2} \times [1 - (x/6)(3+s)]^{1/2} \rightarrow (\hbar/2)(3\rho U_0/m)^{1/2} k, \quad (56)$$

as $k \rightarrow 0$.

We have previously shown in Ref. 2 that the energy for the elementary excitations reproduces fairly well (to within about 20%) the observed spectrum in helium when the wave vector k is averaged over directions for a bcc lattice, for magnitudes of $k \lesssim 2.2A^{-1}$.

Since the parameter V which measures the attractive interactions does not appear in $\epsilon(k)$, we conclude that the attractive forces do not inhibit the energy spectrum typical of a superfluid. The pressure exerted by the system does depend on the attractive interaction. A strong enough attractive interaction may inhibit the solid-superfluid transition due to the fact that the pressure of the system may go to zero for a density larger than ρ_0 , the density at the transition. The latter does not depend on attractive forces, being given, as Eq. (40) indicates, by the relation

$$x_0 = 2K_0/\rho_0 U_0 = \hbar^2/m\rho_0^{1/3} U_0. \quad (57)$$

In Appendix A we make an improved termination of the Green's-function equations. The improvement is affected by writing an equation of motion for the function $H_2(l, t)$ rather than approximating it in terms of G_1 as in Eq. (31). In this way the system of two coupled equations for G_1 and G_2 is replaced by three coupled equations for G_1 , G_2 , and H_2 . Their solution is shown to yield an expression for the energy where it is clearly seen that the attractive interaction has a negligible effect on the density fluctuations of the system, and the transition is hardly affected, owing to the smallness of the attractive interactions compared with the repulsive forces.

IV. MECHANICAL CONSIDERATIONS

Now it is necessary to obtain the pressure as a function of density to find out if the pressure vanishes while

the system is still in its solid state or not, i.e., to find out if there is a solid-superfluid transition or not.

The pressure will be obtained in the form of an expansion in powers of $x = 2K/\rho U_0$. For this purpose the energy of the system will be first obtained, and from it the pressure making use of the relation

$$P = -(\partial E/\partial V)_s. \quad (58)$$

It should be noted that one is dealing with ground-state energies in this problem, therefore the entropy s is zero for all values of the volume. The energy is given by

$$E = \langle \phi_0 | H | \phi_0 \rangle = 6iKNG_1(l=0, t=0^-) - iKND_1(l=0, t=0^-) + i\rho(U_0/2)NG_2(l=0, t=0^-) - i\rho(V/2)NH_2(l=0, t=0^-). \quad (59)$$

Using Eq. (25), we can replace G_2 and H_2 in terms of G_1 and D_1 :

$$\rho U_0 G_2(l, t) - \rho V H_2(l, t) = (i(\partial/\partial t) - 6K)G_1(l, t) + KD_1(l, t). \quad (60)$$

The energy may now be expressed in terms of G_1 and $D_1(l, t) = \sum_\delta G_1(l + \delta, t)$ alone:

$$E/N = (-\frac{1}{2}(\partial/\partial t) + 3Ki)G_1(l=0, t=0^-) - (Ki/2) \sum_\delta G_1(\delta, t=0^-). \quad (61)$$

Utilizing our solution for $G_1(k, t)$ given in Eq. (37) we obtain

$$E/N = (1/N) \sum_k a_1^-(k) [K(3-s(k)) + \rho(U_0/2)\nu^-(k)]. \quad (62)$$

Next we expand the quantities $a_1^-(k)$, $\nu^-(k)$ of Eqs. (39) and (43) in powers of x and obtain

$$E/N = 6K + 3\rho V - 6Kx. \quad (63)$$

The kinetic-energy part is easily seen to be

$$T/N = 6K - 12Kx \quad (64)$$

while the potential-energy part is

$$U/N = 3\rho V + 6Kx = 3\rho V + 3x^2\rho U_0. \quad (65)$$

It is shown in the Appendix, with a better approximation procedure of the Green's-functions equations, that

$$6Kx \rightarrow 6Kx(1 + V/U_0). \quad (66)$$

The potential energy is modified to

$$U/N = 3\rho V + 6Kx[1 + V/U_0] = 3\rho V + 3x^2\rho U_0 + 3x^2\rho V, \quad (67)$$

while the kinetic energy goes over into

$$T/N = 6K - 12Kx[1 + V/U_0], \quad (68)$$

and the energy per particle is

$$E/N = 6K + 3\rho V + 3x^2\rho(U_0 - V) - 12xK. \quad (69)$$

The third term on the right-hand side of Eq. (69) represents the influence of the attractive forces on the

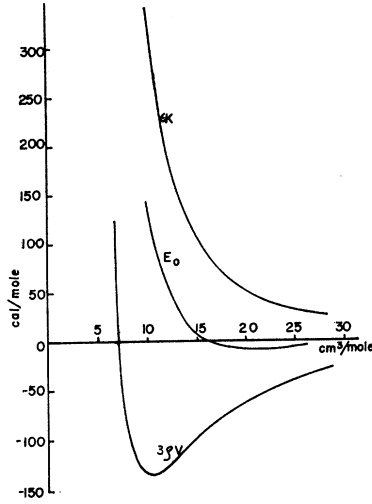


FIG. 2. Graph of the diagonal kinetic energy $6K$ given by Eq. (72) and the lattice potential energy $3\rho V$ given by Eq. (73) as functions of the molar volume of helium in its ground state. The curve marked E_0 is their sum.

density fluctuations. To estimate this influence, we need to know the ratio V/U_0 . The strength of the repulsive interactions U_0 can be estimated by requiring that Eq. (56), which gives the phonon energies for long wavelengths, $\epsilon = \hbar ck$, reproduce the measured sound velocity c at the transition density, $c = 365$ m/sec. In this way, one gets $\rho U_0 \approx 83^\circ\text{K}$. Another estimate of ρU_0 can be obtained by utilizing the definition of the parameter $x = 2K/\rho U_0$. We assume that x_0 at melting density is the same value as previously found, $x_0 = 0.067$. The kinetic energy $6K$ can be estimated from London's expression, Eq. (72) below and Fig. 2. At melting density, corresponding to 21.2 cm³/mole, the kinetic energy is about 42 cal/mole or 21°K per particle.⁵ Then

$$\rho U_0 = 2K/x = (21/3^\circ\text{K})/0.067 \approx 104^\circ\text{K}$$

somewhat higher than the 83°K value obtained from sound velocity. As for the lattice potential energy, London's expression for it given in Eq. (73) below and plotted in Fig. 2 yields $3\rho V = -56$ cal/mole $= -28^\circ\text{K}$ per particle at melting density.⁵ Then, utilizing the smaller of the two estimates in order to maximize the effect of attractive forces, we have, for the ratio V/U_0 ,

$$V/U_0 \approx -9.3/83 \approx -0.1,$$

which is consistent with the value predicted by Eq. (7). It is then clear by inspection of Eq. (69) that the attractive interactions play an almost negligible role in the density fluctuations.

The pressure will be mainly determined by the diagonal energy terms

$$P = \rho^2(\partial(E/N)/\partial\rho) \approx \rho^2(\partial/\partial\rho)(6K + 3\rho V). \quad (70)$$

We want to compare ρ_1 , the density at which the pressure vanishes (for different masses and different

⁵ W. E. Parry, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience Publishers, Inc., New York, 1963). Vol. VI, p. 192, quotes the values $T/N \approx 18^\circ\text{K}$ and $3\rho V \approx -25^\circ\text{K}$ obtained from other considerations.

interaction strengths V) to the density ρ_0 at which there is a transition, given by Eq. (57) as

$$\rho_0 = (\hbar^2/mU_0x_0)^3, \quad (71)$$

with $x_0 \approx 0.067$. To make the comparison quantitatively meaningful, we will use realistic diagonal kinetic energies for K and lattice potentials for V , as given by London in Sec. 5 of his book.³ Our present expression for the diagonal kinetic energy $K = \hbar^2\rho^{2/3}/2m$ is deficient because it does not contain the effects of the hard core, and we will use London's kinetic energy instead [London's Eq. (6)]

$$6K = \frac{\hbar^2\rho^{2/3}}{2m} \rightarrow \frac{2\pi\hbar^2d}{m(R-0.891d)^2(R+0.713d)}, \quad (72)$$

where $R = \rho^{-1/3}$ is the mean atom spacing, and d , which represents the hard sphere diameter, is best chosen at 2.35 Å to fit the experimental density and energy of solid helium, when the potential energy is given by [London's Eq. (14)]:

$$3\rho V \rightarrow (1041e^{-5.3R} - 0.65/R^6 - 0.701/R^8)10^5 \text{ cal/mole}. \quad (73)$$

This potential is obtained by summing over all pairs of close-packed lattice the Yntema-Schneider interaction energy of two helium atoms a distance r away

$$\phi(r) = (1200e^{-4.82r} - 1.24/r^6 - 1.89/r^8) \times 10^{-12} \text{ erg}. \quad (74)$$

Figure 2 shows the diagonal kinetic energy K and potential energy $3\rho V$ given by Eqs. (72) and (73) plotted versus volume per mole. Their sum predicts a zero-pressure density of 27.7×10^{21} particles cm⁻³, the experimental density at 25 atm is 28.4×10^{21} particles cm⁻³.

To investigate the effect of attractive potentials on the possibility of a phase transition, we consider several hypothetical systems having the same mass as helium 4, but with increasing attractive interactions, so that the minimum of the lattice potential energy is a multiple of that for helium. Each such fictitious substance yields increasing density for the zero pressure, approaching the limiting value corresponding to the minimum of the potential energy curve, which is 57.3×10^{21} cm⁻³.

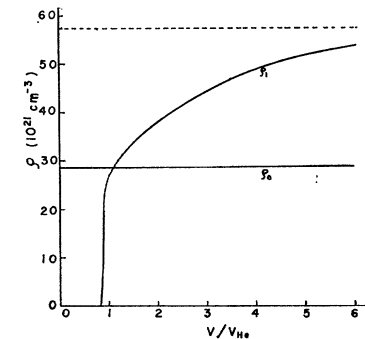
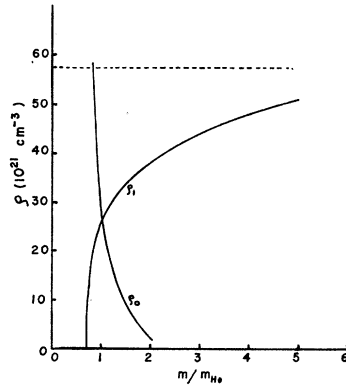


FIG. 3. Graph showing the dependence of ρ_1 , the zero-pressure density, and ρ_0 , the transition density on V/V_{He} , the ratio of attractive interactions to those present in helium, for fixed mass. The dashed line represents the asymptotic value for ρ_1 .

FIG. 4. Graph showing the dependence of the zero-pressure density ρ_1 , and the transition density ρ_0 , on the mass of the Bose systems for fixed interaction strength.



The curve of $\rho(P=0)=\rho_1$ is shown in Fig. 3. The density at the solid-superfluid transition given in Eq. (71) does not depend on the attractive forces and is constant at $\rho_0=28.4 \times 10^{21} \text{ cm}^{-3}$ as shown by the horizontal line in Fig. 3. According to this figure a 15% increase in the strength of attractive interactions over the value for helium four would result in removal of the solid-superfluid transition, since zero pressure would occur before the transition density is reached. Next we consider the effect of the mass of the interacting Bose atoms on the solid-superfluid transition. If we imagine the strength of the attractive interactions V to be constant then the density $\rho(P=0)=\rho_1$ will increase with increasing mass, as shown in Fig. 4. For the transition density ρ_0 , if we imagine bosons with fixed repulsive interactions U_0 and variable mass m , we would have $\rho_0 \sim m^{-3}$ as Eq. (71) indicates. This curve, shown dotted in Fig. 4 would predict a solid-superfluid transition for all such materials of mass less than helium four. However, the real physical Bose system of mass lighter than He is H₂ solid, and in order to realistically compare its possible solid-superfluid transition density with that of helium account must be taken of the changed interactions. These have an effect on both $\rho(P=0)$ and ρ_0 . As far as ρ_0 is concerned, the ratio of the transition densities is more accurately expressed from Eq. (69) as

$$\frac{\rho_0_{\text{H}_2}}{\rho_0_{\text{He}}} = \frac{(mU_0)^3_{\text{H}_2}}{(mU_0)^3_{\text{He}}} = 8 \frac{(U_0)_{\text{H}_2}^3}{(U_0)_{\text{He}}^3}. \quad (75)$$

We can estimate the effect of repulsive forces U_0 from knowledge of the sound velocities c in these solids, since these follow from the dispersion relation $\epsilon = \hbar ck$ and Eq. (56) in the form

$$c = (3\rho U_0/4m)^{1/2} \quad (76)$$

or

$$U_0 = 4c^2 m / 3\rho. \quad (77)$$

We do not know of any sound-velocity measurement in solid hydrogen. However, c has been measured to be

roughly 1300 m/sec in the liquid⁶ and should be about the same in the solid. Sound velocity in helium is about 365 m/sec at melting density.⁷ The densities of solid hydrogen ($\rho \approx 26.5 \times 10^{21} \text{ cm}^{-3}$) and solid helium ($\rho \approx 28.4 \times 10^{21} \text{ cm}^{-3}$) are roughly the same so we obtain the ratio of repulsive interactions in the two systems as

$$U_{0\text{H}_2}/U_{0\text{He}} \cong 2(365/1300)^2 \cong 0.159, \quad (78)$$

and

$$\rho_{0\text{H}_2} \cong 0.03 \rho_{0\text{He}} \cong 0.9 \times 10^{21} \text{ cm}^{-3}. \quad (79)$$

According to this estimate, the increased repulsive interactions in molecular hydrogen far outweigh the effects of the lighter mass, so that the hypothetical solid-superfluid transition in hydrogen would occur at a density of about 0.03 of that in helium.

Next we must know the effect on $\rho(P=0)$ of the interactions present between the H₂ molecules. Here we may quote London's result, that the lattice potential energy in H₂ is given by (London's Eq. 10)

$$\phi_{\text{e.p.}} = (162/R^9 - 9.27/R^6) \times 10^5 \text{ cal/mole}. \quad (80)$$

When this potential is combined with the zero-point kinetic energy for H₂ molecules [Eq. (70) multiplied by a factor of 2], the zero of the pressure occurs at a density of 26×10^{21} particles/cm³, and hence at much greater a density than that of the solid-superfluid density estimated above to be about 1×10^{21} particles/cm³. We conclude that the pressure for H₂ solid will go to zero long before the transition density is reached. The same argument will surely hold for the Bose systems like neon, since they are all heavier and have even stronger interactions than hydrogen.

We conclude by giving another qualitative argument to show that considerations of a strict dynamical character should not lead to a criterion to decide whether a substance is fluid or solid at $T=0$, $P=0$, that depends strongly on the strength of the attractive interactions.

Let a be the width of the two-particle potential interaction well, and let its depth be given by V . If these two particles are free in a large box their energy is about zero. If the two particles are bound together their energy is about $3(\pi^2 \hbar^2 / 2ma^2) - V$. The particles will be free if $3(\pi^2 \hbar^2 / 2ma^2) > V$. The same criterion is sometimes erroneously applied in the case of many particles in a box. If the density of the system in the ground state is very low the energy of a couple of bound particles is about $-V + 3(\pi^2 \hbar^2 / 2ma^2)$, but if the particles are free their energy is about zero plus some small positive contribution from the repulsive interaction with other particles. Let this repulsive interaction be $f(\rho)$ with $df(\rho)/d\rho > 0$. Now consider a couple of particles in a high-density system, i.e., the interatomic distances are

⁶ A. Van Itterbeek, *Physica* **29**, 965 (1963).

⁷ K. R. Atkins, *Liquid Helium* (Cambridge University Press, Cambridge, England, 1959), Chap. 5.

not very much larger than the atomic dimensions. The difference in energy between two systems, one with two particles bound and the other with the two particles free is about $-V + 3(\pi^2 \hbar^2 / 2ma^2) - (-v + \tau + f(\rho))$, where $0 < \tau < 3\pi^2 \hbar^2 / 2ma^2$, $-V < -v < 0$, and $f(\rho) > 0$. We have $\tau > 0$ because the space available for the motion of this particle is not very large due to the presence of the other particles. The quantity $v \neq 0$ because the "free particle" feels the attraction of the other particles in the box to a significant degree due to their closeness. So if $f(\rho) - v + \tau < -V + 3\pi^2 \hbar^2 / 2ma^2$, i.e., $f(\rho) + (V - v) < 3\pi^2 \hbar^2 / 2ma^2 - \tau$, the system will be in a fluid state. The larger the density the more important the role of the repulsive interactions become. For a large enough density $V - v$ becomes negligible, as the results of this paper suggest. For high densities such as those dealt with in this work, a would have to be replaced by a

smaller number, as our "realistic" kinetic energy term in Eq. (72) indicates.

ACKNOWLEDGMENT

We have benefited by numerous discussions of the work reported here with Dr. James M. Tanner.

APPENDIX A

In this Appendix, we show that an improved approximation on the coupled Green's-function equations still shows that the attractive forces have negligible effect on the dynamics of the system.

To improve the results obtained in Sec. III, the last term in Eq. (25) will not be approximated as in Eq. (31); instead, a new equation of motion will be obtained for it:

$$\begin{aligned} (i\partial/\partial t - 6K)H_2(l, t) = & \delta(t)[6\delta_{l,0} + \sum_{\delta} \langle b_{l+\delta}^\dagger b_l \rangle \delta_{l+\delta,0}] \\ & - i\rho V \sum_{\delta', \delta} \langle T b_{l+\delta}^\dagger(t) b_{l+\delta}(t) b_l(t) b_{l+\delta'}^\dagger(t) b_{l+\delta'}(t) b_0^\dagger(0) \rangle - i\rho U_0 \sum_{\delta} \langle T b_{l+\delta}^\dagger(t) b_{l+\delta}(t) b_l^\dagger(t) b_l(t) b_0^\dagger(0) \rangle \\ & - K \sum_{\delta, \delta'} [G(l+\delta, l+\delta, l+\delta') + G(l+\delta, l+\delta+\delta', l) + G(l+\delta+\delta', l+\delta, l)], \quad (A1) \end{aligned}$$

in which

$$G(l, m, p) = -i \langle T b_l^\dagger(t) b_m(t) b_p(t) b_0^\dagger(0) \rangle. \quad (A2)$$

In order to truncate the system of equations we make the following approximations, which are all asymptotically exact in the limit of high densities:

$$-i \sum_{\delta} \langle T b_{l+\delta}^\dagger(t) b_{l+\delta}(t) b_l^\dagger(t) b_l(t) b_0^\dagger(0) \rangle \cong 6G_2(l, l), \quad (A3)$$

$$-i \sum_{\delta} \langle T b_{l+\delta}^\dagger(t) b_{l+\delta}(t) b_l(t) b_{l+\delta'}^\dagger(t) b_{l+\delta'}(t) b_0^\dagger(0) \rangle \cong H_2(l, t), \quad (A4)$$

$$\sum_{\delta'} G(l+\delta, l+\delta, l+\delta') \cong \sum_{\delta' \neq \delta} G_1(l+\delta', l) + G(l+\delta, l+\delta, l+\delta), \quad (A5)$$

$$\sum_{\delta'} G(l+\delta, l+\delta+\delta', l) = (g/6) \sum G_1(l+\delta+\delta', l), \quad (A6)$$

$$\sum_{\delta'} G(l+\delta+\delta', l+\delta, l) \cong (1-1/6)gG_1(l, l) + G_1(l+\delta, l), \quad (A7)$$

where

$$g = \sum_{\delta} \langle b_{l+\delta}^\dagger b_l \rangle. \quad (A8)$$

The equation for H_2 can now be written in the form

$$\begin{aligned} (i\partial/\partial t - 6K - 6\rho V)H_2(l, t) = & \delta(t)[6\delta_{l,0} + \sum_{\delta} \langle b_{l+\delta}^\dagger b_l \rangle \delta_{l+\delta,0}] + 6\rho U_0 G_2(l, t) \\ & - (Kg/6) \sum_{\delta, \delta'} G_1(l+\delta+\delta', t) + 5gKG_1(l, t) + K \sum_{\delta} G_1(l+\delta, t) - 6K \sum_{\delta' \neq \delta} G_1(l+\delta', t) - K \sum_{\delta'} G_2(l+\delta', t). \quad (A9) \end{aligned}$$

Comparing Eqs. (33) and (A9), one notices that for $x=0$, $H_2=6G_1$, which is the approximation used in Sec. III

for H_2 . Now solving Eqs. (33), (34), and (A9) for $G_1(l, t)$, one obtains

$$\begin{aligned} & (i\partial/\partial t - 6K)(i\partial/\partial t - 6K - 6\rho V)(i\partial/\partial t - 6K - 6\rho V - \rho U_0)G_1(l, t) \\ &= \delta_{l,0}(i\partial/\partial t - 6K - 6\rho V)(i\partial/\partial t - 6K - \rho U_0 - 6\rho V)\delta(t) - (i\partial/\partial t - 6\rho V)(i\partial/\partial t - 6K - 6\rho V - \rho U_0)K \sum_{\delta'} G_1(l + \delta', t) \\ & \quad + \rho U_0(i\partial/\partial t - 6K)[2\delta_{l,0} - 2K \sum_{\delta'} G_1(l + \delta', t) + KgG_1(l, t)] + \rho V(i\partial/\partial t - 6K - 6\rho V - \rho U_0) \\ & \quad \times [6\delta_{l,0}\delta(t) + g\delta(t) - (Kg/6) \sum_{\delta, \delta'} G_1(l + \delta + \delta', t) + 5KgG_1(l, t) + K \sum_{\delta} G_1(l + \delta, t) - 6K \sum_{\delta' \neq \delta} G_1(l + \delta', t)] \\ & \quad - KV[2\delta(t) - 2K \sum_{\delta, \delta'} G_1(l + \delta + \delta', t) + K \sum_{\delta'} g(\delta')G_1(l + \delta, t)], \quad (\text{A10}) \end{aligned}$$

where

$$g(\delta') = \sum_{\delta} \langle b_{l+\delta+\delta'}^\dagger b_l \rangle.$$

An expression for the energy will be obtained now. We first compute the value $h = \sum_{\delta} \langle b_l^\dagger b_{l+\delta} \rangle$. Let

$$G_1(l, t) = \sum_{n=0}^{\infty} K^n G_1^{(n)}(l, t). \quad (\text{A11})$$

Substituting this expression into Eq. (A10), one obtains, after some simplification, an equation for $G_1^{(0)}$:

$$(\omega - 6K - 6\rho V)(\omega - 6K - 6\rho V - \rho U_0)G_1^{(0)}(l, \omega) = \delta_{l,0}(\omega - 6K - 6\rho V + \rho U_0). \quad (\text{A12})$$

The solution to this equation is

$$G_1^{(0)}(l, \omega) = \delta_{l,0} \left[-\frac{1}{(\omega - 6K - 6\rho V - i\eta)} + \frac{2}{(\omega - 6K - 6\rho V - \rho U_0 + i\eta)} \right]. \quad (\text{A13})$$

Let

$$A(\omega) = -\frac{1}{(\omega - 6K - 6\rho V - i\eta)} + \frac{2}{(\omega - 6K - 6\rho V - \rho U_0 + i\eta)}. \quad (\text{A14})$$

Then

$$G_1^{(0)}(l, \omega) = \delta_{l,0} A(\omega).$$

The next equation obtained relates $G_1^{(0)}(l, \omega)$ and $G_1^{(1)}(l, \omega)$:

$$\begin{aligned} & (\omega - 6K)(\omega - 6K - 6\rho V)(\omega - 6K - 6\rho V - \rho U_0)G_1^{(1)}(l, \omega) \\ & + \sum_{\delta} G_1^{(0)}(l + \delta, \omega) [(\omega - 6K - 6\rho V)(\omega - 6K - 6\rho V - \rho U_0) + 2\rho U_0(\omega - 6K) \\ & \quad - \rho V(\omega - 6K - 6\rho V - \rho U_0)] = \rho V(\omega - 6K - 6\rho V - \rho U_0)(h^{(1)}/6) \sum_{\delta} \delta_{l+\delta,0}, \quad (\text{A15}) \end{aligned}$$

where

$$h^{(1)} = iD_1^{(1)}(l=0, t=0^-).$$

It follows from Eq. (A15) that

$$\begin{aligned} G_1^{(1)}(l, \omega) = & -A^2(\omega) \sum_{\delta} \delta_{l+\delta,0} + \frac{6\rho VA(\omega) \sum_{\delta} \delta_{l+\delta,0}}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho V - i\eta)} \\ & + \frac{\rho V(h^{(1)}/6) \sum_{\delta} \delta_{l+\delta,0}}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho V - i\eta)} - 4\rho VA(\omega) (\sum_{\delta} \delta_{l+\delta,0})^2. \quad (\text{A16}) \end{aligned}$$

It follows from Eq. (A13) that

$$iD_1^{(0)}(l=0, t=0^-) = h^{(0)} = 0, \quad (\text{A17})$$

and

$$h^{(1)} = \frac{i}{2\pi} \int D_1^{(1)}(l=0, \omega) e^{-i\omega 0^-} d\omega. \quad (\text{A18})$$

From (A16) it follows that

$$h^{(1)} = \frac{i}{2\pi} \int \left[-A^2(\omega) + \frac{\rho V}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho V - i\eta)} (2A(\omega) + h^{(1)}) \right] e^{-i\omega 0^-} d\omega. \quad (\text{A19})$$

Now

$$-\frac{i}{2\pi} \int A^2(\omega) e^{-i\omega 0^-} d\omega = 24/\rho U_0, \quad (\text{A20})$$

and

$$\begin{aligned}
& \frac{i}{2\pi} \int \frac{2\rho V A(\omega) e^{-i\omega 0^-}}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho V - i\eta)} d\omega \\
&= \frac{i}{2\pi} 2\rho V \int \frac{1}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho V - i\eta)} \left[-1 + \frac{2}{(\omega - 6K - 6\rho V - \rho U_0 + i\eta)} \right] e^{-i\omega 0^-} d\omega \\
&= \frac{i}{2\pi} \int \left[\frac{1}{6\rho V(\omega - 6K - 6\rho V - i\eta)} - \frac{1}{6\rho V(\omega - 6K - i\eta)} - \frac{1}{(\omega - 6K - 6\rho V - i\eta)^2} \right. \\
&\quad \left. + \frac{12\rho V}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho V - i\eta)(\omega - 6K - 6\rho V - \rho U_0 + i\eta)} \right] e^{-i\omega 0^-} d\omega. \quad (A21)
\end{aligned}$$

The previous expression equals

$$-\frac{1}{6\rho V} + \frac{1}{6\rho V} + \frac{12\rho V}{6\rho^2 V U_0} - \frac{12\rho V}{6\rho V(\rho U_0 + 6\rho V)} \sim \frac{12\rho V}{(\rho U_0)^2}. \quad (A22)$$

Also

$$\int \frac{h^{(1)} \rho V e^{-i\omega 0^-}}{6(\omega - 6K - i\eta)(\omega - 6K - 6\rho V - i\eta)} d\omega = 0. \quad (A23)$$

Therefore,

$$h^{(1)} = \frac{24}{\rho U_0} + \frac{24\rho V}{(\rho U_0)^2}, \quad (A24)$$

but

$$h = h^{(0)} + K h^{(1)},$$

so

$$h = 12x(1 + V/U_0). \quad (A25)$$

Now we are ready to find an expression for the energy of the system. From Eq. (61), which is exact, and Eqs. (A11) and (A25) one can write

$$\frac{E}{N} = \frac{i}{2\pi} \int \frac{\omega}{2} [G_1^{(0)}(l=0, \omega) + K G_1^{(1)}(l=0, \omega)] e^{-i\omega 0^-} d\omega + 3K - 6Kx(1 + V/U_0), \quad (A26)$$

where only the first two terms in the expansion of G_1 , were used. Now it is clear by inspection of Eq. (A16) that

$$\int \frac{\omega}{2} G_1^{(1)}(l=0, \omega) e^{-i\omega 0^-} d\omega = 0. \quad (A27)$$

The only task to be performed now is the evaluation of the integral

$$\int \frac{\omega}{2} G_1^{(0)}(l=0, \omega) e^{-i\omega 0^-} d\omega. \quad (A28)$$

Substituting Eq. (A12) we obtain

$$\int \frac{\omega}{2} G_1^{(0)}(l=0, \omega) e^{-i\omega 0^-} d\omega = -2\pi i(3K + 3\rho V). \quad (A29)$$

It follows, then, that the energy per particle is given by

$$E/N = 6K + 3\rho V - 6Kx(1 + V/U_0). \quad (A30)$$

This appears in the text as Eq. (69). Now the kinetic energy T is

$$T/N = 6K - 12Kx(1 + V/U_0) \quad (A31)$$

as follows from Eqs. (4) and (A25). This relation for kinetic energy appears as Eq. (68) in the text. We also get

$$U/N = (E - T)/N = 3\rho V + 3x^2(\rho U_0 + \rho V) \quad (A32)$$

which is Eq. (67) in the text.