Simplified Model of Liquid Helium

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A simplified version of a Bose gas with negative scattering length is studied with a model Hamiltonian similar to that used in the case of repulsive interactions. A new transformation is used which takes into account the attractive interactions in the system, and the ground-state energy is calculated from experimental values of the sound velocity in the system. Real values for the phonon energy spectrum are obtained, and the ratio of the effective mass to ordinary mass is deduced using experimental values of interparticle separation and core radius. A justification for using this modified Hamiltonian is attempted in the Appendix.

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m ECENTLY^{1-7}}$ an intensive study of the Bose gas has been made using various methods of approach such as the pseudopotential method, linked-cluster expansion method, the transformation techniques, and the propagator formalism. But most of the results obtained so far are confined to a system of a Bose gas with repulsive interactions for which one has positive twobody scattering length only.

It will be the purpose of this paper to examine the consequences in the case in which there is a predominantly repulsive interaction with negative scattering length. The situation corresponds to the actual liquid helium in which particles are interacting with a shallow attractive potential with hard-core repulsion inside. We examine the system under the following assumptions: that the bare potential which appears in the Hamiltonian describing the system can be replaced in some way (which we do not know exactly at present) with a smeared out K matrix (or pseudopotential) which has a definite low momentum limit, and secondly, that even after the replacement, the system can be described by the Schrödinger equation with a Hamiltonian which we call a model Hamiltonian.

In the following, we first seek a possible model Hamiltonian which corresponds to the case of liquid helium. Eventually, we arrive at the same model Hamiltonian wich was used before in the case of positive scattering length (low-density limit). It is well known that if we merely replace the sign of the scattering length in the results for phonon excitation energy usually obtained in the case of positive scattering length, applying the transformation proposed by Bogoliubov,³ we are led to complex (nonreal) excitation energy, which means that the system is unstable. This shows the necessity of redistribution of particles among the various states in the "free" wave function, contrary to the ordinary treatment for the case of positive scattering length in which one assumes that in the "free" wave function all the particles are sitting in the momentum-zero state, that this state is sufficiently rigid, and that a perturbation cannot change the state drastically. We perform this redistribution by using a canonical transformation which mixes momentum-zero states and finite-momentum states, and fix the mixing parameter by requiring the energy to be minimum in the Hartree-Fock sense. Finally, we apply to the transformed model Hamiltonian the Bogoliubov transformation and show that the phonon excitation is in fact real for negative scattering length.

Let us begin by writing down the usual Hamiltonian in the second quantized version as

$$\sum_{q} \frac{q^{2}}{2m} \beta_{q}^{\dagger} \beta_{q} + \frac{1}{2} n_{0} (n_{0} - 1) v_{0} + \sum_{q} n_{q} (v_{q} + v_{0}) n_{0}$$

$$+ \frac{1}{2} \sum_{q} \beta_{q}^{\dagger} \beta_{-q}^{\dagger} v_{q} \beta_{0} \beta_{0} + \text{c.c.}$$

$$+ \sum_{p} \sum_{q} \beta_{q}^{\dagger} \beta_{p}^{\dagger} \frac{1}{2} (v_{p} + v_{q}) \beta_{p+q} \beta_{0} + \text{c.c.}$$

$$+ \frac{1}{2} \sum_{p} \sum_{p'} \sum_{q} \beta_{p+q}^{\dagger} \beta_{p'}^{\dagger} v_{q} \beta_{p'+q} \beta_{p}. \quad (1)$$

(Sums do not include momentum zero.) In the above, β_q and β_q^{\dagger} are, respectively, the boson annihilation and creation operators, the q's are the particle momenta, and $n_0 = \beta_0^{\dagger} \beta_0, n_q = \beta_q^{\dagger} \beta_q$ are number operators.

Under the assumptions we have made and by the reasoning we are going to present in the following, we would like to examine the system with a model Hamiltonian given by

$$H_{\text{model}} = \sum_{q} (q^{2}/2m)\beta_{q}^{\dagger}\beta_{q} + \frac{1}{2} \left(\alpha - \alpha \sum_{q} \frac{1}{-2\epsilon_{q}} \alpha \right) n_{0}(n_{0}-1)$$
$$+ \sum_{q} n_{q} 2\alpha n_{0} + \frac{1}{2} \sum_{q} \beta_{q}^{\dagger}\beta_{q}^{\dagger}\alpha\beta_{0}\beta_{0} + \text{c.c.}, \quad (2)$$
$$\epsilon_{q} = q^{2}/2m,$$

where α is the scattering K matrix and is taken as constant neglecting momentum dependence (i.e., we consider only low-momentum excitation) as well as density dependence.

First of all, the model Hamiltonian (2) is the same as the Hamiltonian used (in the low-density limit) when the scattering length is positive ($\alpha = 4\pi a/m\Omega$; a is the

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⁷ K. Sawada, Phys. Rev. 119, 2090 (1960).

scattering length and Ω is the normalization volume of the system).^{1–7}

In the case of α being negative, we have sufficient reasons to argue that (2) may describe the system. Firstly, we cannot include the type of interactions which have the form of the last two terms of (1) in the model Hamiltonian (2) which is supposed to describe liquid helium, because if we do so, the energy of the system becomes proportional to (number of particles)^{1+ β} (β >0) times a constant (density-dependent) which is of order one. Hence we are led to a lack of saturation of energy as is shown in Appendix A. [Note that we have neglected and actually do not claim to know in this paper the density dependence of α in (2); hence we cannot discuss the existence of a saturating density. The latter, namely, the existence of a minimum in the density-energy diagram, is also another assumption we have made. On the other hand, the terms in the model Hamiltonian (2) give as the energy of the system a quantity proportional to the number of particles times a constant (density-dependent) which is of order one (see Appendix A). We also show in Appendix C that there can be a few other possible terms which can be added to our model Hamiltonian leading to saturation in the same sense as above, but the conclusions obtained therefrom are quite similar to those obtained in the following by using (2) only.

These arguments on the justification of (2) as model Hamiltonian are not very strong and, of course, depend on the assumptions we have made. But in this paper we shall regard (2) as our basic Hamiltonian and proceed to obtain a few results.

There have been different ways used to treat the system with the Hamiltonian (2). In the variational treatment, in the case of positive α , the type of trial state vector employed in earlier work is

 $|0\rangle = C \exp[A] \phi_0$

where

$$A = \frac{1}{2} g_0 \beta_0^2 + \sum_k g_k \beta_k^{\dagger} \beta_k^{\dagger}, \qquad (4)$$

(3)

and C is the normalization constant; g_0, g_k are variational parameters, and ϕ_0 represents the free ground state in which all particles are sitting in momentumzero state. Using the state vector (3) is equivalent to the application of the well-known Bogoliubov transformation U to (2), where

$$U = \exp\left[-\sum_{k} g_{k} (\beta_{k}^{\dagger} \beta_{-k}^{\dagger} - \beta_{-k} \beta_{k})\right], \qquad (5)$$

and the determination of g_k by minimizing the constant terms obtained after transforming the Hamiltonian.

It is well known that, if we use the above technique in the case of negative α , we obtain the complex (nonreal) phonon excitation energy. This points out the inadequacy of taking ϕ_0 as the free ground state.

To incorporate the attractive interaction which changes the occupation of particles (especially those between the zero-momentum state particles and the excited ones), we transform the state vector by a different unitary operator,

$$U_1 = \exp\left[-\sum_k f_k (\beta_k^{\dagger} \beta_0 - \beta_0^{\dagger} \beta_k)\right], \qquad (6)$$

where f_k is an arbitrary parameter (mixing parameter) to be determined later. The one-particle wave function corresponding to this will no longer be a plane wave but a distorted one as it should be.

We see that

$$U_{1}\beta_{k}^{\dagger}U_{1}^{-1} = \beta_{k}^{\dagger} + s_{k} [\sum_{k'} s_{k'}\beta_{k'}^{\dagger}(u_{0}-1) - v_{0}\beta_{0}^{\dagger}], \quad (7)$$

$$U_{1}\beta_{0}^{\dagger}U_{1}^{-1} = u_{0}\beta_{0}^{\dagger} + v_{0}\sum_{k}s_{k}\beta_{k}^{\dagger}, \qquad (8)$$

where

and

$$v_0 = \sin\{(\sum_k f_k^2)^{\frac{1}{2}}\}.$$

 $s_k = f_k / (\sum_{k'} f_{k'}^2)^{\frac{1}{2}}; \quad u_0 = \cos\{ (\sum_k f_k^2)^{\frac{1}{2}} \},\$

Similarly, the transformations for β_k and β_0 are, respectively, the complex conjugates of Eqs. (7) and (8).

To fix the variational parameter f_k , we evaluate the ground-state energy by transforming the model Hamiltonian (2) by the operator U_1 and picking out the diagonal terms after replacing β_0 and β_0^{\dagger} by the *C* number $\sqrt{N_0}$, where N_0 is the number of particles in the zero-momentum state. (After transformation, we suppose that the "free" ground state is sufficiently rigid, whereby $N_0 \approx N$, the total number of particles.)

Applying the transformations given by Eqs. (7) and (8) to the terms of the model Hamiltonian (2), we find the leading diagonal terms to be

$$E^{(1)} = E_{a}{}^{(1)} + E_{b}{}^{(1)},$$

$$E_{a}{}^{(1)} = \sum_{q} v_{0}{}^{2}s_{q}{}^{2}N_{0}\epsilon_{q} + 2\alpha \sum_{q} v_{0}{}^{2}s_{q}{}^{2}N_{0}{}^{2}u_{0}{}^{2}$$

$$+ \frac{1}{2}\alpha u_{0}{}^{4}N_{0}{}^{2} + \sum_{q} s_{q}{}^{2}v_{0}{}^{2}u_{0}{}^{2}N_{0}{}^{2}, \quad (10)$$

$$E_{b}{}^{(1)} = -\frac{1}{2}\alpha \sum_{q} \frac{1}{-2\epsilon_{q}} \alpha u_{0}{}^{4}N_{0}{}^{2}.$$

Besides taking α to be a constant, we also make the following simplifying assumptions: We take the quantity f_q to be a constant for $q < q_{\text{max}}$ and 0 for $q > q_{\text{max}}$ (with $\sum_q f_q^2$ being of order one for the transformation to be nontrivial), and write

$$\sum_{q < q_{\max}} s_q^2 \epsilon_q = \bar{\epsilon}.$$

As a result of these simplifications, we arrive at an expression for the ground-state energy $E_a^{(1)}$ [obtained by transformation of (2) by U_1]:

$$E_{a}^{(1)} = -\frac{5}{2}\alpha N_{0}^{2} \left\{ \cos^{2} \left[\left(\sum_{k} f_{k}^{2} \right)^{\frac{1}{2}} \right] - \frac{3\alpha N_{0} - \bar{\epsilon}}{5\alpha N_{0}} \right\}^{2} + \bar{\epsilon} N_{0} + \frac{(3\alpha N_{0} - \bar{\epsilon})^{2}}{10\alpha N_{0}} N_{0}.$$
(11)

(9)

Here we do not include $E_b^{(1)}$ to the variational procedure to find a suitable f_k which makes the energy of the system a minimum, assuming that α is a small quantity and hence treating $E_b^{(1)}$ as a higher order correction.

For a negative value of the scattering K matrix α , the minimization condition leads to

$$\cos^{2}\left[\left(\sum_{k} f_{k}^{2}\right)^{\frac{1}{2}}\right] = (3\alpha N_{0} - \bar{\epsilon})/5\alpha N_{0}.$$
(12)

Then $E_a^{(1)}$ is determined in terms of the parameter $\bar{\epsilon}$:

$$E_a^{(1)} = \bar{\epsilon} N_0 + \frac{(3\alpha N_0 - \bar{\epsilon})^2}{10\alpha N_0} N_0.$$
(13)

The limits of $\bar{\epsilon}$, which is to be always positive, are set by the condition (12) and the fact that α is negative. Hence

$$0 < \bar{\epsilon} < -2\alpha N_0. \tag{14}$$

In view of this, the minimum energy is obtained when $\bar{\epsilon}=0$, and this immediately determines the value $\cos^2\left[\left(\sum_k f_k^2\right)^{\frac{1}{2}}\right]$ to be $\frac{3}{5}$. The minimum value of the ground-state energy is

$$E_{a}^{(1)} = \frac{9\alpha N_{0}^{2}}{10} = -\frac{1}{2}(9/5) |\alpha| N_{0}^{2}, \qquad (15)$$

and this is less than $-\frac{1}{2}|\alpha|N_0^2$ as it should be. The fact that $\bar{\epsilon}$ is to be zero restricts the number of particles involved in the transformation U_1 in higher momentum states to almost zero. Considering the fact that $\bar{\epsilon}=0$ while $\cos^2[(\sum_k f_k^2)^{\frac{1}{2}}]$ has to be $\frac{3}{5}$, we can determine f_q as

$$f_q = f/(4\pi M^3)^{\frac{3}{2}}, \quad 0 < q < 2\pi M/L \quad (16)$$

= 0, $2\pi M/L < q.$

[M is some arbitrary number (>0 and finite) and L is the dimension of the quantization box.] Here f_q is replaced by the $f_{|q|}$ since the angular dependence of f_q is the same for all values of \mathbf{q} .

Equation (16) gives $\bar{\epsilon}=O(1/L^2) \rightarrow 0$ as $L \rightarrow \infty$. This shows that only in the immediate neighborhood of q=0are particles excited. Our next task is to look for the existence of the phonon spectrum and study the various features of these excitations. In all previous work, a negative scattering length has led to the difficulty of complex energy values for the low-lying excitations. We shall see, after applying the transformation U_1 (6), that our transformed (model) Hamiltonian becomes

$$H_{T} = \sum_{q} \left(\frac{q^{2}}{2m} + (6/5)\alpha n_{0} \right) \beta_{q}^{\dagger} \beta_{q} + \left[\frac{1}{2} \frac{3}{5} \alpha \sum \beta_{q}^{\dagger} \beta_{q}^{\dagger} \beta_{0} \beta_{0} + \text{c.c.} + \text{terms which contain } \sum_{q} f_{q} s_{q} \beta_{q} \right]$$
(17)

+
$$\left[\frac{1}{2}\alpha(9/5)n_0(n_0-1)-\frac{1}{2}\alpha\sum_{q}\frac{1}{-2\epsilon_q}\alpha(\frac{3}{5})^2n_0(n_0-1)\right],$$

where we have used $\cos^2\left[\left(\sum_q f_q^2\right)^{\frac{1}{2}}\right] = \frac{3}{5}; \ \bar{\epsilon} = 0.$

To calculate the single-particle excitation energies in our case, we use the method of the equation of motion.⁷ We take the commutator of the single-particle (approximate) eigenmode operator X_{-q}^* with our transformed Hamiltonian, where X_{-q}^* is given by

$$X_{-q}^* = [\chi_{-q}\beta_{-q}^* + \beta_q \psi_q].$$
⁽¹⁸⁾

This procedure, as explained elsewhere, will lead to the determination of ω_q , the single-particle excitation energies of momentum q, and is equivalent to making a further transformation [namely, Bogoliubov transformation (5)] to our once transformed Hamiltonian (17). The relevant eigenvalue equation (in the Heisenberg representation) will be

$$[X_q^*, H_T] = -\omega_q X_q^* + Y_q.$$
⁽¹⁹⁾

If we choose V_q as a small quantity, ω_q , χ_q , and ψ_q are to be determined by the eigenvalue equation.

In applying this method to our system, we have to remember that since the Bogoliubov transformations do not conserve the number of particles, we have to replace $n_0 = \beta_0^{\dagger} \beta_0$ by $N - \sum_q n_q$, in all the terms.⁸ This, of course, does not affect the ground-state energy obtained earlier $(E_a^{(1)}, E_b^{(1)})$. But we have a term

$$-\alpha N \sum_{q} (9/5) n_q, \tag{20}$$

which arises from the first term inside the last square bracket in Eq. (17). This in turn adds to the coefficient of the $\beta_q^{\dagger}\beta_q$ term in (17). With regard to other terms in (17) above, the replacement is equivalent to replacing β_0 and β_0^{\dagger} by \sqrt{N} .

$$H_T = \sum_{q} \left[\frac{q^2}{2m} + \left(-\frac{3}{5} \alpha N \right) \right] \beta_q^{\dagger} \beta_q$$
$$+ \frac{1}{2} \left(\frac{3}{5} \alpha N \right) \sum \beta_q^{\dagger} \beta^{q\dagger} + \text{c.c.}$$
$$+ (\text{terms which contain } \sum f_q S_q^{n} \beta_q)$$

 $E_a^{(1)} = \frac{1}{2}\alpha(9/5)N^2$

where

$$+E_{a}^{(1)}+E_{b}^{(1)}+\Delta \mathcal{E},$$
 (21)

$$E_b^{(1)} = -\frac{1}{2} \left(\frac{3}{5}\right)^2 \alpha N \sum_q \frac{1}{-2\epsilon_q} \alpha N, \qquad (22)$$

$$\Delta \mathcal{E} = \left(\frac{3}{5}\right)^2 \alpha N \sum_q \frac{1}{-2\epsilon_q} \alpha \sum_q n_q.$$

We regard $\Delta \mathcal{E}$ as a perturbation to the "gap" $\left(-\frac{3}{5}\alpha N\right)$ and discard it from the present discussion.⁸

With the transformed model Hamiltonian (21) the commutator of Eq. (19) for finite values of q yields

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⁸ Strictly speaking, we had to use the procedure similar to Hugenholtz and Pines, Phys. Rev. 116, 489 (1959); Sec. 4 of reference 6. The procedure is explained in Appendix B together with the meaning of $\Delta \mathcal{E}$ (22) which we have omitted from our discussion.

the result,

$$\begin{bmatrix} X_{-q}^*, H_T \end{bmatrix} = \beta_q \{ \psi_q [\epsilon_q + (-\frac{3}{5}\alpha N)] - \frac{3}{5}\alpha N \chi_{-q} \} \\ + \beta_{-q}^* \{ -\chi_{-q} [\epsilon_q + (-\frac{3}{5}\alpha N)] + \frac{3}{5}\alpha N \psi_q \}.$$
(23)

Besides these terms, we have for the commutator terms of the following types:

$$\begin{split} \psi_{q}s_{q}\epsilon_{q}\sum s_{k}\beta_{k}\times \text{constant terms,} \\ s_{q}\psi_{q}\sum s_{k}\beta_{k}\times \text{constant terms,} \\ s_{q}^{n}\psi_{q}\sum s_{k}\beta_{k}\times \text{constant terms,} \\ s_{q}\psi_{q}\sum s_{k''}\sum s_{k}\beta_{k}\times \text{constant terms.} \end{split}$$
(24)

In addition there are terms which are bilinear in the operators which we neglect here. In the expression (24) the quantity s_q defined by Eq. (9) tends to zero for finite values of q by virtue of (16).

Since we are interested only in the energy eigenvalue of the single-particle excitations, we can neglect these scattering terms. However, if there appears a resonance between single-particle states and collective oscillations in the system, then the scattering terms will become highly important in determining the normal modes. But we drop them for simplicity.

Hence, the single-particle eigenvalue equation to be solved can be written as

$$-\omega_{q}[\beta_{q}\psi_{q}+\beta_{-q}^{*}\chi_{-q}] = \beta_{q}\{\psi_{q}[\epsilon_{q}+(-\frac{3}{5}\alpha N)]-\frac{3}{5}\alpha N\chi_{-q}\} + \beta_{-q}^{*}\{-\chi_{-q}[\epsilon_{q}+(-\frac{3}{5}\alpha N)]+\frac{3}{5}\alpha N\psi_{q}\}.$$
 (25)

We can deduce from Eq. (25) that the single-particle energy eigenvalue is

$$\omega_q = \left[\epsilon_q^2 + 2\epsilon_q \left(-\frac{3}{5}\alpha N\right)\right]^{\frac{1}{2}}.$$
(26)

[The result is, of course, the same as what we would get if we applied the Bogoliubov transformation to the first two terms in (21).] For small values of $q \ (q \rightarrow 0)$, we get the phonon spectrum

$$\omega_q = q \left[(1/m) \left(-\frac{3}{5} \alpha N \right) \right]^{\frac{1}{2}}.$$
(27)

For negative α , this yields real energy values for phonon excitations. We should note here that the spectrum (26) is obtained from our model Hamiltonian in which we have neglected the momentum dependence of the scattering K matrix completely (low-momentum approximation), and hence (26) is only valid for the socalled phonon region. For higher momentum excitations, particularly near the roton region, we would expect the repulsive hard core to play a dominant role and the momentum dependence of the K matrix to become very important.¹

The eigensolutions (in the approximation we are considering) for ψ_q and χ_q can also be derived easily and from the fact that X_q, X_q^* obey Bose commutation relations, we are able to normalize them and obtain

the following:

where

$$\begin{aligned} \psi_q &= \frac{3}{5} \alpha N / [2\omega_q(\omega_q + \tilde{\epsilon}_q)]^{\frac{1}{2}}, \\ \chi_{-q} &= (\omega_q + \tilde{\epsilon}_q) / [2\omega_q(\omega_q + \tilde{\epsilon}_q)]^{\frac{1}{2}}, \end{aligned} \tag{28}$$

 $\tilde{\epsilon}_q = \epsilon_q + (-\frac{3}{5}\alpha N).$

We shall now turn our attention to getting the correction to the ground-state energy of our system, incorporating the Bogoliubov transformation (5) within the approximation in which we neglect effect of "terms" which contain $\sum f_q \beta_q$ and $\Delta \mathcal{E}$ from (21), by arguing in the same way as we did in the case of the single-particle energy. [We can evaluate the energy by using the inverse expressions for β_q and β_q^* in terms of the X_q 's, putting them into (21), and introducing an ordering about X_q, X_q^* , but here we use the Bogoliubov transformations for convenience.]

The operator U transforms the creation and annihilation operators in the manner shown below

$$U\beta_k^{\dagger}U^{-1} = (\beta_k^{\dagger} \cosh g_k - \beta_{-k} \sinh g_k). \tag{30}$$

We apply this transformation to Eq. (21) and minimize the energy obtained by collecting the diagonal terms. This variational procedure gives for $\cosh g_k$ and $\sinh g_k$ the values

$$\begin{aligned} \cosh g_k &= (\omega_k + \tilde{\epsilon}_k) / [2\omega_k(\omega_k + \tilde{\epsilon}_k)]^{\frac{1}{2}},\\ \sinh g_k &= \frac{3}{5} \alpha N / [2\omega_k(\omega_k + \tilde{\epsilon}_k)]^{\frac{1}{2}}. \end{aligned} \tag{31}$$

Using the above, we find the energy of the system to be given by

$$UU_{1}HU_{1}^{-1}U^{-1}$$

$$=E_{a}^{(1)}+E_{b}^{(1)}+\sum_{q}\omega_{q}\beta_{q}^{\dagger}\beta_{q}$$

$$+\frac{1}{2}(\frac{3}{5})^{2}\alpha N\sum_{q}\frac{1}{-\omega-\tilde{\epsilon}_{q}}\alpha N$$
(32)

 $+U(\text{terms which contain } \sum f_q \beta_q S^n \text{ and } \Delta \mathcal{E})U^{-1}.$

The constant terms which yield the ground-state energy can be written as

$$E_{0} = \frac{1}{2} \left(\frac{3}{5} \alpha N \right) 3N + \frac{1}{2} \left(\frac{3}{5} \alpha N \right)^{2} \left(\sum_{q} \frac{1}{-\omega_{q} - \tilde{\epsilon}_{q}} - \sum_{q} \frac{1}{-2\epsilon_{q}} \right), \quad (33)$$

with ω_q , $\tilde{\epsilon}_q$ given by (26) and (29).

This energy expression is of the same form as we get by applying the Bogoliubov transformation only to (2) if $\alpha > 0$ except for the replacement of α by $\frac{3}{5}\alpha$ and a multiplicative factor 3 in the first-order energy. For $\alpha > 0$, the Bogoliubov transformation yields

$$E_0 = \frac{1}{2} (\alpha N) N + \frac{1}{2} (\alpha N)^2 \left[\sum_q \frac{1}{-\omega_q - \tilde{\epsilon}_q} - \sum_q \frac{1}{-2\epsilon_q} \right],$$

with

$$\omega_q = (\epsilon_q^2 + 2\alpha \epsilon_q N)^{\frac{1}{2}}$$
 and $\tilde{\epsilon}_q = \epsilon_q + \alpha N$.

(29)

If we define the scattering length *a* by $\alpha = 4\pi a/m\Omega$ and $N/\Omega = \rho$, the density of the system, we get the familiar form for the energy with a few changes;

$$E_{0} = -N \frac{2\pi\rho}{m} \bigg[3\left| \frac{3}{5}a \right| - \frac{128}{15\sqrt{\pi}} \left| \frac{3}{5}a \right|^{\frac{5}{2}} \rho^{\frac{1}{2}} \bigg].$$
(34)

It is now interesting to examine how well our results derived above for the ground-state energy, etc., agree with the experimental data relating to liquid helium. From the vapor pressure curves for helium the ground-state energy is deduced as -13.2 cal/mole,⁹ though different types of experiments allow considerable latitude to this figure. The above value corresponds to an energy of $(-5.715) \times 10^{-4}$ electron volt per particle. The sound velocity *C* in the system can be derived from Eq. (27), and since the experimental value for *C* is 237 meters/sec, we can write

$$\left[\frac{3}{5}\frac{\left[-\alpha(0)\right]}{m^*}N\right]^{\frac{1}{2}} = C = 237 \times 10^2, \tag{35}$$

where, instead of m, we used m^* which is the effective mass for low-lying excitations of the system. The first order ground-state energy from Eq. (11) is therefore expressed in terms of the ratio (m^*/m) as

$$E^{(1)} = 3.485 \times 10^{-3} \times (m^*/m) \text{ ev.}$$
 (36)

A method to find m^* is to look into the term $\sum n_q(v_q+v_0)n_0$ of our Hamiltonian (1) and find out the excess contribution to the single-particle energy if we have not substituted $\alpha(0)$ for $\alpha(q)$ as we have done in this paper. Since $\alpha(q)$ can be related to $\alpha(0)$ for small momentum transfers as

$$\alpha(q) = \alpha(0) + q^2 \frac{\partial \alpha}{\partial q^2} \bigg|_{q=0} = \alpha + q^2 \Delta$$
(37)

the altered single-particle energy becomes

$$\omega_{q} = \left[\left(\frac{q^{2}}{2m} + \frac{3}{5} N_{0} q^{2} \Delta - \frac{3}{5} N \alpha \right)^{2} - \left(\frac{3}{5} N \alpha \right)^{2} \right]^{\frac{1}{2}}.$$
 (38)

The effective-mass equation is therefore given by

$$\frac{1}{2m^*} = \frac{1}{2m} + \frac{3}{5}N\Delta.$$

Since the core radius is of order 2.6 A, we can expect the $\alpha(q)$ to change its sign at a value q_0 which is of order $\hbar/(2.6 \text{ A})$ because at momentum zero, the scattering length is negative and at momentum higher than $\approx (\hbar/2.6 \text{ A}), \alpha(q)$ is to be positive. Hence Δ can be expressed in terms of $\alpha(0)$ which in turn has been obtained from the sound velocity Eq. (35) as a function

of m^* . A few algebraic operations lead to a quadratic equation for the ratio (m/m^*) :

$$\left(\frac{m}{m^*}\right)^2 = \left(\frac{m}{m^*}\right) + 2\frac{237^2 \times 10^4}{q_0^2}m^2,$$
 (39)

where $q_0 \approx \hbar/2.6 \times 10^{-8}$ and *m* is the mass of He⁴. This yields a value for m^*/m of

$$m^*/m = 0.165.$$

Hence, our first-order ground-state energy from Eq. (36) is

$$E^{(1)} = -5.75 \times 10^{-4} \text{ ev}, \tag{40}$$

which is comparable to the experimental result. We can proceed further to calculate the second-order energy assuming an interparticle separation of 3.6 A, and obtain the ratio (using m^* instead of m for the ϵ_q 's)

$$E^{(2)}/E^{(1)} = -0.107. \tag{41}$$

The smallness of this ratio will assure us that the energy expression we have obtained is meaningful. Finally, from the relation which can hold between α and the scattering length a,

$$\alpha = 4\pi a/m^*\Omega$$
,

we find *a* to be of order of -2 A.

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APPENDIX A

If in the Hamiltonian of Eq. (1) we assume a constant attractive interaction α , apply the transformation (5), and collect the leading contributions to the groundstate energy, the last term gives a factor of the form

$$\frac{1}{2}\alpha \sum_{p} \sum_{p'} \sum_{q} s_{p+q} s_{p'} s_{p'+q} s_{p} v_0^4 N_0^2.$$
 (A-1)

Since, for the transformation to be nontrivial, $\sum_{k} k_{k}^{2}$ is to be of order 1, and $N_{0} \sim \Omega$ and $\alpha \sim 1/\Omega$, this term, when α is negative, immediately leads to failure of saturation in the system since it is proportional to $-N^{3}|\alpha|$, where N is the number of particles in the system. In an analogous way the terms of the Hamiltonian

$$\sum_{q} \sum_{p} \alpha \beta_{p}^{\dagger} \beta_{q}^{\dagger} \beta_{p+q} \beta_{0} + \text{c.c.}$$

present us with leading contributions of the form

$$-\alpha \sum_{p} \sum_{q} u_{0} v_{0}^{2} N_{0}^{2} s_{p+q} s_{p} s_{q}.$$
 (A-2)

This also results in the system becoming unsaturated. The above also implies that u_0 is so chosen to be negative and v_0 to be positive or vice versa. It can easily be seen that the other terms of the Hamiltonian lead to a saturating system.

The justification for studying the system with the last two terms of the Hamiltonian removed (as has

⁹ K. A. Atkins, *Liquid Helium* (Cambridge University Press, New York, 1959).

been done in this paper) may be grasped if we try to construct the K matrix of the system with a mainly positive interaction (v>0), but with a negative scattering length a<0. In this procedure, we will see that the last two terms in the Hamiltonian (1) which cause the processes represented in Fig. 1, modify the rest of the terms of the Hamiltonian. Hence, we can take as our model Hamiltonian

$$H^{(1)} = \sum_{q} \frac{q^{2}}{2m} \beta_{q}^{*} \beta_{q} + \frac{1}{2} v_{0} n_{0} (n_{0} - 1) + \sum_{q} 2\alpha n_{q} n_{0} + \frac{1}{2} \alpha \sum_{q} \beta_{q}^{\dagger} \beta_{q} \beta_{0} \beta_{0} + \text{c.c.} \quad (A-3)$$

a



FIG. 1. Diagrams showing effects of last two terms in the Hamiltonian (1) on the others, γ is the momentum of the excited particle.

To obtain the above, we consider α in (11) as a K matrix obtained by summing diagrams in Fig. 2 and omitting the momentum dependence of α_1 and α_2 for simplicity. We note here that $H^{(1)}$ defined in (A-3) must be supplemented by a term

$$H^{(2)} = -lpha \sum_{q} \left(rac{1}{-2\epsilon^{q}}
ight) lpha eta_{0}^{\dagger} eta_{0}^{\dagger} eta_{0} eta_{0} + v_{0} \sum_{q} rac{1}{-2\epsilon^{q}} lpha eta_{0}^{\dagger} eta_{0} eta_{0} eta_{0}.$$
 (A-4)

The addition of this can be accounted for in the following manner. The second order correction to the first order energy obtained from (A-3) is given by



FIG. 2. K matrix for forward scattering and for pair creation.



FIG. 3. Second order diagram in α obtained from (A-3).

which is represented in Fig. 3; but in inserting this term we are overcounting some of the contributions from the diagram one would obtain from the Hamiltonian (1). The original Hamiltonian gives second order contributions to the energy which can be represented by summing up the diagrams of Fig. 4 in which the first interaction point is to be a v_0 interaction instead of α interaction. Hence, $H^{(2)}$ supplements $H^{(1)}$ to give the correct result. By adding (11) and (12), and using

$$\alpha = v_0 + v_0 \sum_{q} \left(-\frac{1}{2\epsilon^q} \right) \alpha, \qquad (A-5)$$

we get as our model Hamiltonian

FIG. 4. Diagram obtained from (1) representing two-particle scattering.

It is obvious from our observations for attractive interactions that H_{model} for a saturating system with negative scattering length should not have interactions of the form represented by the last two terms of Eq. (1) which we have included in the K matrix. Hence, it can be said generally that the model Hamiltonian is to be of the form (2).

APPENDIX B

The procedure to be used in a more rigorous treatment for the system with the Hamiltonian (17) is to replace n_0 by a number \overline{N} which is determined by the condition

$$N = \overline{N} + (\overline{\psi}_{\overline{N}}, \sum_{k} n_{k} \overline{\psi}_{\overline{N}}). \tag{B-1}$$

Here $\bar{\psi}_{\bar{N}}$ is the eigensolution of the equation

and

$$\begin{bmatrix} H_T(\bar{N}) - \mu \sum_k n_k \end{bmatrix} \bar{\psi}_{\bar{N}} = E_{\bar{N}} \bar{\psi}_{\bar{N}}, \qquad (B-2)$$

$$\mu = \partial E_{\bar{N}} / \partial \bar{N}. \tag{B-3}$$

The ground-state energy becomes

$$E_0 = E_{\overline{N}} + \mu(\bar{\psi}_{\overline{N}}, \sum n_k \bar{\psi}_{\overline{N}}). \tag{B-4}$$

Taking the definition of μ given in (B-3), if we assume for the energy $E_{\overline{N}}$ the approximate value given by the last two terms in the square bracket of Eq. (17) with n_0 replaced by \overline{N} , we see that

$$\mu = \frac{\partial}{\partial \bar{N}} E_N \approx \frac{\partial}{\partial \bar{N}} \left[\frac{1}{2} \alpha \bar{N}^2 (9/5) - \frac{1}{2} (\frac{3}{5})^2 \alpha \bar{N} \sum_q \frac{1}{-2\epsilon_q} \alpha \bar{N} \right]$$
$$= \mu^{(1)} + \mu^{(2)}.$$

where $\mu^{(1)}$ is given by

$$-\mu^{(1)}\sum_{k}n_{k}=-\alpha\bar{N}\sum_{q}(9/5)n_{q},$$

which is the same expression as Eq. (20), and $\mu^{(2)}$ by

$$-\mu^{(2)}\sum_k n_k = \Delta \mathcal{E},$$

where $\Delta \mathcal{E}$ is the same quantity found in Eq. (22). Then the Hamiltonian $[H_T(\bar{N}) - \mu \sum_k n_k]$ in Eq. (B-2) becomes exactly the same as our model Hamiltonian (27) except for the fact that N is replaced by \bar{N} .

We have discarded the quantity $\Delta \mathcal{E}$ from our discussions in the text. Here we find that $\Delta \mathcal{E}$ is a part of the second order chemical potential $\mu^{(2)}$. But this $\mu^{(2)}$ is really to be derived from the actual value of E_N taken up to the second order, which is the equation for E_0 given by expression (33) in the text. If we do so, we find that the divergences in $\mu^{(2)}$ arising from the differentiation and summing up of the second order terms cancel each other. It is easy to see that $\Delta \mathcal{E}$ is the contribution obtained by differentiation of the second order factor containing the term $\sum [1/(-2\epsilon_q)]$ in Eq. (33). The other second order factor, which is the result of the Bogoliubov transformation, after differentiation yields another divergent term similar to $\Delta \mathcal{E}$.

Hence in all our expressions in the text \tilde{N} given by (B-1) should replace N. To calculate the quantity \tilde{N} , we can use Eq. (B-1) and obtain

$$N = \bar{N} + 2.8 (m^*/m)^3 \bar{N} = \bar{N} \times 1.013.$$
 (B-5)

In evaluating the above we have used the approximation that $\bar{\rho} \approx \rho$ which, in view of the small depletion effect indicated by (B-5), is a good approximation.

It is interesting to observe that while the result (B-5) shows that the mean number of particles in the excited states, corresponding to the situation represented by the transformed Schrödinger wave function, is very small, the mean number of excited particles corresponding to the original untransformed Schrödinger wave function, namely the quantity $(\psi, \sum_k n_k \psi)$ where ψ is the eigensolution of the equation $H_{model}\psi = E\psi$, is not so small. To estimate this wave function ψ we take the transformed model Hamiltonian and remove the interaction terms therefrom. Then the wave function ψ should correspond to the Hamiltonian represented by Eq. (17) without the terms in the square bracket and

hence is approximately the free ground-state wave function. We can write

$$\psi = U_1^{-1} \phi_0.$$

Hence the number of particles in nonzero momentum states is given by

$$(\phi_0, U_1 \sum_k n_k U_1^{-1} \phi_0) = v_0^2 \sum_k s_k^2 N = \frac{2}{5} N. \quad (B-6)$$

In determining the above we have made use of Eqs. (7) and (8) and taken the value of $\cos^2\left[\left(\sum_k f_k^2\right)^{\frac{1}{2}}\right]$ to be $\frac{3}{5}$.

APPENDIX C

On the basis of the arguments employed in Appendix A to analyze the saturating properties of the various terms of the Hamiltonian (1), and in view of the structure of our transformation U_1 which mixes the excited states with zero-momentum states in a nontrivial way, we would like to point out that after eliminating the nondiagonal (scattering) interaction terms (by incorporating them suitably into the K matrix which is not achieved here) there remain, in addition to the terms found in our model Hamiltonian (2), a few other terms which even with a negative scattering length for the interaction lead to the saturation of the system in the sense of Appendix A.

These additional terms are

$$H_{\text{model}}^{(1)} = \alpha \sum_{qq'} \beta_q^{\dagger} \beta_{q'}^{\dagger} \beta_{q'} \beta_q + \frac{\alpha}{2} \sum_{qq'} \beta_q^{\dagger} \beta_{-q}^{\dagger} \beta_{q'} \beta_{-q'}. \quad (C-1)$$

The corresponding diagrams representing these interaction terms are given in Fig. 5. But in taking our Hamiltonian as $H_{\text{model}}+H_{\text{model}}^{(1)}$ we are committing the error of overcounting some of the processes of second order represented by the diagrams given in Fig. 6. Hence, to evaluate energies correctly up to second order we should delete these processes from the interaction; this can be done by adding to the Hamil-



FIG. 5(a). Diagram showing forward scattering of excited particles. (b) Diagram for pair to pair scattering.



FIG. 6. Second order diagrams in α obtained from (A-3) and (C-1) together which appear in addition to diagrams in Fig. 3.

tonian a supplementary term $H_{\text{model}}^{(2)'}$:

$$H_{\text{model}}^{(2)'} = -\frac{1}{2} \alpha \sum_{q''} \frac{1}{-2\epsilon_{q''}} \alpha \sum_{qq'} \beta_q^{\dagger} \beta_q^{\dagger} \beta_{q'} \beta_{q'}$$
$$-\frac{1}{2} \alpha \sum_{q''} \frac{1}{-2\epsilon_{q''}} \alpha \sum_{q} (\beta_q^{\dagger} \beta_{-q}^{\dagger} \beta_0 \beta_0 + \text{c.c.}). \quad (C-2)$$

We apply now the transformation U_1 to the total Hamiltonian, $H_{\text{model}}+H_{\text{model}}{}^{(1)'}+H_{\text{model}}{}^{(2)'}$, and pick out the leading diagonal terms. After that we use the variational procedure. This leads to the following conditions:

$$\cos^{2}[(\sum_{k} f_{k}^{2})^{\frac{1}{2}}] = 0, \quad \tilde{\epsilon} = 0;$$
 (C-3)

and the minimum energy itself becomes

$$E_a^{(1)} = \frac{1}{2} \alpha N_0^2 \times 3.$$
 (C-4)

In arriving at this value, we have as a first approximation discarded the second order $E_b^{(1)}$ terms [Eq. (10)] and similar terms obtained from $H_{\text{model}^{(2)'}}$. Also we have made variations of the parameter f_k only.

The total transformed Hamiltonian can be written as

 $H_{\mathrm{transformed}}$

$$= U_{1}(H_{\text{model}} + H_{\text{model}}^{(1)\prime} + H_{\text{model}}^{(2)\prime})U_{1}^{-1}$$

$$= \sum \frac{q^{2}}{2m} n_{q} + \frac{1}{2} \alpha (\sum \beta_{q}^{\dagger} \beta_{-q}^{\dagger} \beta_{0} \beta_{0} + \text{c.c.})$$

$$+ 2\alpha n_{0} \sum_{q} n_{q} + \frac{1}{2} \times 3\alpha n_{0}^{2} - \frac{1}{2} \alpha \sum_{q'} \frac{1}{-2\epsilon_{q'}} \alpha n_{0}^{2}$$

$$+ (\text{terms which contain } \sum_{q} f_{q} \beta_{q} s_{q}). \quad (C-5)$$

The above expression is just the same as Eq. (17) obtained by transforming the first term H_{model} only by the operator U_1 , except for the fact that the term $\frac{3}{5}\alpha$ in (17) is replaced by α here.

Hence, in this case also, all our previous results calculated with H_{model} alone follow in exactly the same way with the only change mentioned above. Since we have used the value of the phonon velocity determined experimentally to calculate the energies, etc., the numerical values arrived at earlier remain unchanged.