Hard-Sphere Approach to the Excitation Spectrum in Liquid Helium II*

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The excitation spectrum of a Bose system of hard spheres is obtained in a high-density calculation including multiple scattering processes. The hard-sphere interaction is represented by a non-Hermitian pseudopotential constructed in a previous work, and the T-matrix method of Brueckner and Sawada is adopted with modifications to take into account the non-Hermitian property of the Hamiltonian. The inclusion of multiple scattering is found essentially to give a screening effect to the two-body interaction in a many-body medium. The screening factor is studied within certain approximations and is shown to play a very important role in determining the shape of the excitation spectrum. The effect of depletion of particles from the zero-momentum state due to particle interaction is also included in a self-consistent way and is found to be very small. The calculated spectrum is then applied to liquid helium and there is a good qualitative agreement with experiments. Especially, a roton-type dip exists in the spectrum.

I. INTRODUCTION

THE problem of elementary excitations in liquid helium II was first attacked by Landau,[1] who postulated the existence of phonons and rotons from a study of its thermodynamic behavior. The general features of the excitation spectrum proposed by Landau have been borne out by subsequent experiments including a recent direct measurement of Henshaw and Woods[2] from inelastic neutron scatterings.

As Landau's phenomenological treatment is not satisfactory from the theoretical point of view, many authors have attempted to derive the spectrum from first principles. Feynman,[3] and later Feynman and Cohen,[4] assumed a variational wave function and derived a spectrum in fairly good agreement with experiments. However, a more rigorous approach by statistical calculations using a model interatomic potential is desirable. Work along this line was first initiated by Bogoliubov,[5] and later extensively developed by Lee, Huang, and Yang.[6] But all these calculations are valid only for a system with density much lower than that of liquid helium, and the spectrum they obtained consists only of the phonon part.

Brueckner and Sawada[7] (B-S) applied the Lippmann-Schwinger[8] T-matrix method to a hard-sphere boson system with high density, and made a calculation of the spectrum which is in fair qualitative agreement with the experimental results. However, they did not allow for the depletion of the zero-momentum state due to particle interaction. Parry and Ter Haar[9] included this depletion effect under the B-S framework and found that the dispersion curves no longer bend over; thus, even the qualitative agreement with experiments achieved by B-S is lost in a more careful consideration. In addition, if an attractive tail is added to the hard core, even poorer agreement was found. Hence, Parry and Ter Haar concluded that the hard-sphere boson gas is not by any means as good a model for liquid helium as has been assumed. However, their conclusion is based on the treatment of the hard-sphere interaction by B-S as a screened delta-function potential. In other words, their hard spheres can still penetrate into each other and the effect of this penetration in a boson system has not been investigated.

To represent the nonpenetrating hard spheres, we (LL and KWW) constructed a two-body pseudopotential in a previous work.[10] This potential was then used to evaluate both the ground-state energy and the excitation spectrum for a dilute Bose system. The spectrum obtained then had a good resemblance to the Landau's curve after we made the following unjustified assumptions: The formula of the spectrum derived for the low-density gas is applicable to liquid helium, but due to multiple scatterings in such a dense medium the interaction strength is expected to increase and thus was arbitrarily boosted to make the slope of the spectrum at $k=0$ compatible with the measured sound velocity.

In this paper we like to report a calculated excitation spectrum for a high-density system. The hard-sphere interaction, which represents the core part of the interaction potential between two helium atoms, is replaced

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by a two-body pseudopotential discussed in Ref. 10. The T matrix, as developed by B-S, is adopted with modifications to take into account our non-Hermitian potential. It is found that the inclusion of multiple scatterings in the T matrix gives essentially an enhancement to the effective two-body interaction in a many-body medium. Thus, the excitation spectrum obtained has the same analytical form as the one we derived for the low-density gas in Ref. 10, but the parameter characterizing the interaction strength does get enhanced. In other words, the arbitrary assumptions we made are justified by the present investigation.

The effect of depletion of particles from the zero-momentum state due to particle interaction is also taken into account in a self-consistent manner and is found to be very small. The spectrum using the parameters pertinent to liquid helium agrees qualitatively well with the experiments even after the depletion effect is included.

The paper is organized into six sections. The next section gives the effective Hamiltonian in terms of T matrix. The integral equation of the T matrix is then solved for hard spheres in Sec. III, which also contains a study of the screening factor. Section IV treats the depletion effect. The excitation spectrum using parameters pertinent to liquid helium is studied in Sec. V and the last section involves a general discussion.

II. EFFECTIVE HAMILTONIAN WITH T MATRIX

We start with the second-quantized Hamiltonian of a system of interacting bosons enclosed in a box of volume Ω.

$$H=\sum_{\mathbf{k}}(\hbar^2k^2/2m)a_{\mathbf{k}}{}^*a_{\mathbf{k}} +\tfrac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} V_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4}a_{\mathbf{k}_1}{}^*a_{\mathbf{k}_2}{}^*a_{\mathbf{k}_3}a_{\mathbf{k}_4}, \quad (2.1)$$

where $a_{\mathbf{k}}{}^*$ and $a_{\mathbf{k}}$ are the creation and annihilation operators of a boson with mass m and momentum $\hbar\mathbf{k}$. $V_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4}$ is the matrix element of the two-body potential taken with respect to a basis set of plane-wave states,

$$\begin{aligned}V_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4}&=\frac{1}{\Omega^2}\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 e^{-i\mathbf{k}_1\cdot\mathbf{x}_1}e^{-i\mathbf{k}_2\cdot\mathbf{x}_2} \times V\left(r,\frac{\partial}{\partial r}\right)e^{i\mathbf{k}_3\cdot\mathbf{x}_1}e^{i\mathbf{k}_4\cdot\mathbf{x}_2}\\ &=\frac{1}{\Omega}\delta_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4}\int d^3\mathbf{r}e^{-i\frac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{r}} \times V\left(r,\frac{\partial}{\partial r}\right)e^{i\frac{1}{2}(\mathbf{k}_3-\mathbf{k}_4)\cdot\mathbf{r}}, \quad (2.2)\end{aligned}$$

where $\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$ is the relative coordinate between the two particles at positions $\mathbf{x}_1$ and $\mathbf{x}_2$, and the Kronecker delta function $\delta_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4}$ expresses the conservation of total momentum.

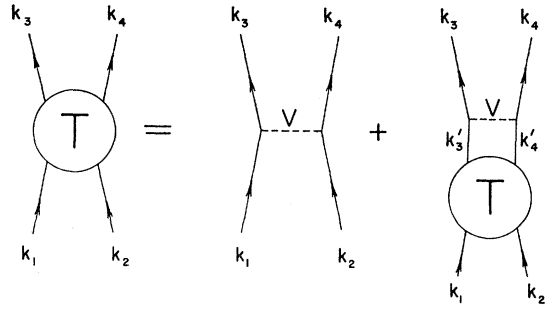

FIG. 1. Graphical representation of the T-matrix equation. The interaction V is represented by dashed lines.

In our previous work on dilute gas,[10] we replaced the creation and annihilation operators for zero-momentum states, $a_0{}^*$ and a_0, in (2.1) by a c number, and diagonalized the part of Hamiltonian bilinear in $a_{\mathbf{k}}{}^*$ and $a_{\mathbf{k}}$ by a Bogoliubov[5] transformation to get the ground-state energy and the excitation spectrum. In perturbational language, this procedure is equivalent to summing up diagrams in the random-phase approximation. However, for a high-density system, we have to go beyond the random-phase approximation and take into account more diagrams describing multiple scatterings. We do this by following B-S, and express the result in terms of an effective Hamiltonian,

$$\begin{aligned}H_{\text{eff}}&=\tfrac{1}{2}N_0(N_0-1)T_{00,00}\\ &+\sum_{\mathbf{k}\neq 0}\{[(\hbar^2k^2/2m)+N_0(T_{0\mathbf{k},0\mathbf{k}}+T_{0\mathbf{k},\mathbf{k}0}-T_{00,00})]\\ &\times a_{\mathbf{k}}{}^*a_{\mathbf{k}}+\tfrac{1}{2}N_0(T_{\mathbf{k}-\mathbf{k},00}a_{\mathbf{k}}{}^*a_{-\mathbf{k}}{}^* +T_{00,\mathbf{k}-\mathbf{k}}a_{\mathbf{k}}a_{-\mathbf{k}})\}, \quad (2.3)\end{aligned}$$

which contains the occupation number in zero-momentum state, N_0, as a result of replacing $a_0{}^*$ and a_0 in H by $(N_0)^{1/2}$. In (2.3) the Lippmann-Schwinger scattering matrix T plays the role of an effective interaction, and it satisfies the integral equation,

$$T_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4}=V_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3\mathbf{k}_4} +\sum_{\mathbf{k}_3'\mathbf{k}_4'}V_{\mathbf{k}_1\mathbf{k}_2,\mathbf{k}_3'\mathbf{k}_4'}G(\mathbf{k}_3'\mathbf{k}_4',\mathbf{k}_3\mathbf{k}_4)T_{\mathbf{k}_3'\mathbf{k}_4',\mathbf{k}_3\mathbf{k}_4}, \quad (2.4)$$

where G is the propagator for the intermediate pair of particles. To facilitate easy visualization, a diagramatic representation of the T-matrix equation is given in Fig. 1.

In general, a Hamiltonian of the form of (2.3), which is bilinear in $a_{\mathbf{k}}{}^*$ and $a_{\mathbf{k}}$ can be diagonalized by a Bogoliubov[5] transformation

$$\begin{aligned}b_{\mathbf{k}}&=(1-\alpha_{\mathbf{k}}{}^2)^{-1/2}(a_{\mathbf{k}}+\alpha_{\mathbf{k}}a_{-\mathbf{k}}{}^*),\\ b_{-\mathbf{k}}&=(1-\alpha_{\mathbf{k}}{}^2)^{-1/2}(a_{-\mathbf{k}}+\alpha_{\mathbf{k}}a_{\mathbf{k}}{}^*),\end{aligned} \quad (2.5)$$

with a proper choice of the parameter α_k. However, H_{eff} in (2.3) may not be Hermitian if we are going to use a non-Hermitian pseudopotential for V. To deal with a non-Hermitian Hamiltonian, we follow Wu's[11] method in considering the expectation value with respect to a left-hand state vector different from the right-hand counterpart, each determined by a different α_k. For the right state, α_k is chosen to be

$$\alpha_k=\frac{(\hbar^2k^2/2m)+N_0T_k}{N_0T_{00,k-k}}\times\left\{1-\left[1-\frac{N_0^2T_{k-k,00}T_{00,k-k}}{[(\hbar^2k^2/2m)+N_0T_k]^2}\right]^{1/2}\right\}, \quad (2.6)$$

where T_k is a short-hand notation for the following combination of T-matrix elements

$$T_k\equiv T_{0k,0k}+T_{0k,k0}-T_{00,00}. \quad (2.7)$$

For the left state, $\bar{\alpha}_k$ is given by the same expression (2.6), only with $T_{00,k-k}$ and $T_{k-k,00}$ interchanged, or

$$\bar{\alpha}_k=(T_{00,k-k}/T_{k-k,00})\alpha_k. \quad (2.8)$$

With the distinction of left and right states, we write down the part of H_{eff} which gives nonvanishing ex-expectation values with respect to left and right Bogoliubov states,

$$H_{\text{eff}}=E_0+\sum_{k\neq0}E_{ex}(k)b_k^*b_k. \quad (2.9)$$

The ground-state energy E_0 and the excitation spectrum $E_{ex}(k)$ are given in terms of the T-matrix elements as follows:

$$E_0=\tfrac{1}{2}N_0(N_0-1)T_{00,00}+\tfrac{1}{2}\sum_{k\neq0}[(\hbar^2k^2/2m)+N_0T_k]\times\left\{-1+\left[1-\frac{N_0^2T_{k-k,00}T_{00,k-k}}{[N_0T_k+(\hbar^2k^2/2m)]^2}\right]^{1/2}\right\}, \quad (2.10)$$

and

$$E_{ex}(k)=[(N_0T_k+(\hbar^2k^2/2m))^2-N_0^2T_{k-k,00}T_{00,k-k}]^{1/2}. \quad (2.11)$$

Now, we only have to solve for the T matrix in order to obtain the excitation spectrum.

III. T MATRIX FOR HARD SPHERES

For two-body hard-sphere interaction, we can replace the boundary condition imposed on the two-particle wave function by a pseudopotential introduced in Ref. 10,

$$V\left(r,\frac{\partial}{\partial r}\right)=\lim_{\epsilon\to0}(\hbar^2/ma)\delta(r-a)((\partial/\partial r)r)_{r=a+\epsilon}, \quad (3.1)$$

where a is the diameter of the hard sphere and ϵ is a *positive* infinitesimal quantity. Note that the Dirac δ function is centered at $r=a$ while the derivative is to be evaluated at $r=a+\epsilon$. We refer to Ref. 10 for the construction of this pseudopotential and to Sec. VI of the present paper for a discussion concerning its validity.

The matrix element of $V(r,(\partial/\partial r))$ can be evaluated straightforwardly from (2.2), and it depends only on the relative momentum. Introducing $\frac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)=\mathbf{k}'$, $\frac{1}{2}(\mathbf{k}_3-\mathbf{k}_4)=\mathbf{k}$ and dropping the Kronecker delta function, we obtain

$$V_{k',k}=\sum_{l=0}^{\infty}(2l+1)V_l(k,'k)P_l(\hat{k}'\cdot\hat{k}),$$

$$V_l(k,'k)=(4\pi\hbar^2a/m\Omega)j_l(k'a)\times[j_l(ka+k\epsilon)+k(a+\epsilon)j_l'(ja+k\epsilon)], \quad (3.2)$$

where j_l is the spherical Bessel function and j_l' is its first derivative with respect to its argument, and P_l is the Legendre polynomial.

We substitute this hard-sphere potential into the integral equation for the T matrix in (2.4) and try to find its solution. Since the propagator for the intermediate pair of particles, G, in (2.4) depends on the difference between the energies of the intermediate and the initial states of such a pair, which in turn depend on the T matrix, the equation is a complicated nonlinear integral equation. However, it can be solved if we make certain approximations concerning G, which will be stated as we go along.

We follow B-S and assume that the motion of the center of mass of the pair in G can be separated. This approximation should be very accurate as long as the relative momentum of the typical excited state is large compared to the total momentum. Parry and Ter Haar[9] actually performed some calculations and their results seem to suggest that this center-of-mass approximation is unlikely to cause a large error. Using this approximation and relative momenta $\mathbf{k}$, $\mathbf{k}'$ and $\mathbf{k}''=\frac{1}{2}(\mathbf{k}_3'-\mathbf{k}_4')$, we can rewrite (2.4) as

$$T_{k',k}=V_{k',k}+\sum_{k''}V_{k',k''}G(\mathbf{k}'',\mathbf{k})T_{k'',k}. \quad (3.3)$$

Based on the fact that our partial-wave matrix element $V_l(k',k)$ in (3.2) is separable in k' and k, we make a partial-wave decomposition of $T_{k',k}$ which is also separable in k' and k as follows:

$$T_{k',k}=\sum_{l=0}^{\infty}(2l+1)j_l(k'a)T_l(k)P_l(\hat{k}'\cdot\hat{k}). \quad (3.4)$$

Substituting this into (3.3) with $\sum_{k''}$ replaced by a corresponding integration over k'', and assuming no angular correlation between $\mathbf{k}$ and $\mathbf{k}''$ in $G(\mathbf{k}'',\mathbf{k})$, we

[11] T. T. Wu, Phys. Rev. **115**, 1390 (1959).

obtain

$$T_l(k)=N_l(k)/D_l(k),$$
$$N_l(k)=\frac{4\pi\hbar^2 a}{m\Omega}[j_l(ka+k\epsilon)+k(a+\epsilon)j_l'(ka+k\epsilon)], \quad (3.5)$$
$$D_l(k)=1-\frac{\Omega}{2\pi^2}\int_0^\infty dk'k'^2 j_l(k'a)N_l(k')G(k',k).$$

From (3.4) and (3.5) we obtain the solution for the T matrix,

$$T_{\mathbf{k}',\mathbf{k}}=\sum_{l=0}^{\infty}(2l+1)\frac{V_l(k',k)}{D_l(k)}P_l(\hat{k}'\cdot\hat{k}), \quad (3.6)$$

and $D_l(k)$ can now be written simply as

$$D_l(k)=1-\frac{\Omega}{(2\pi)^3}\int d^3\mathbf{k}'V_l(k',k')G(k',k). \quad (3.7)$$

The physical meaning of Eq. (3.6) is very transparent; the two-body partial-wave potential $V_l(k',k)$ given in Eq. (3.2) is screened in a many-body medium by a screening factor $D_l(k)$. Now our problem of solving the T matrix is reduced to finding a solution for this screening factor.

If we further replace the pair propagator $G(k',k)$ according to B-S by a propagator $G(k')$ with the two particles taken initially from the zero-momentum state,

$$G(k')=-[2N_0T_{k'}+(\hbar^2k'^2/m)]^{-1}, \quad (3.8)$$

then the screening factor D_l becomes momentum-independent.

The combination of the T-matrix elements $T_{\mathbf{k}}$ involved in $G(k)$ now takes the form

$$T_{\mathbf{k}}=\frac{4\pi\hbar^2 a}{m\Omega}\left\{\sum_{l=\text{even}}2(2l+1)\frac{j_l(\frac{1}{2}ka)}{D_l}[j_l(\tfrac{1}{2}ka+\tfrac{1}{2}k\epsilon)+\tfrac{1}{2}k(a+\epsilon)j_l'(\tfrac{1}{2}ka+\tfrac{1}{2}k\epsilon)]-(1/D_0)\right\}. \quad (3.9)$$

Hereafter, we shall make an approximation that D_l is independent of angular momentum and is replaced by its s-wave value, or $D_l\simeq D_0$. This has been shown by B-S to be a good replacement at high density in connection with a similar quantity. This simple replacement allows us to perform the summation over l in (3.9) and the result is

$$T_{\mathbf{k}}=\frac{2\pi\hbar^2 a}{m\Omega}\frac{1}{D_0}\left(\frac{\sin ka}{ka}+\cos ka\right). \quad (3.10)$$

In (3.10) we have already taken the limit $\epsilon\to 0$, and this will not affect any of our later results. Substituting (3.10) into (3.8) gives

$$G(k)=-\left[\frac{\hbar^2k^2}{m}+\frac{\hbar^2k_0^2}{2mD_0}\left(\frac{\sin ka}{ka}+\cos ka\right)\right]^{-1}, \quad (3.11)$$

where k_0^2 is defined as

$$k_0^2\equiv 8\pi a\rho_0, \quad (3.12)$$

with

$$\rho_0\equiv N_0/\Omega. \quad (3.13)$$

Then, Eq. (3.7) with $l=0$ constitutes an equation for D_0,

$$D_0=1+\lim_{\epsilon\to 0}\frac{2a}{\pi}\int_0^\infty dk \times\left(k^2\frac{\sin ka}{ka}\cos k(a+\epsilon)\Big/\left[k^2+\frac{k_0^2}{2D_0}\left(\frac{\sin ka}{ka}+\cos ka\right)\right]\right). \quad (3.14)$$

We should point out that the limit $\epsilon\to 0$ and the integration in Eq. (3.14) can not be interchanged. Treating the limiting process carefully, we can rewrite Eq. (3.14) in terms of the following dimensionless quantities,

$$x\equiv ka,$$
$$x_0\equiv k_0a, \quad (3.15)$$
$$\Lambda^2\equiv x_0^2/D_0,$$

as

$$\frac{x_0^2}{\Lambda^2}=\tfrac{1}{2}+\frac{1}{\pi}\int_0^\infty dx\frac{x\sin 2x}{x^2+\frac{1}{2}\Lambda^2((\sin x/x)+\cos x)}. \quad (3.16)$$

This equation expresses Λ^2, or the screening factor D_0, as a function of $a^3\rho_0$. The integrand in the above integral is regular so long as $\Lambda^2\lesssim 20$ and can be evaluated numerically; the results are given in Fig. 2. The value of D_0 in the present approximation is nearly 0.5 for all densities except zero density (for which $D_0\to 1$) as deduced from Fig. 2. In other words, the effective two-particle interaction strength is almost doubled when they are put into a many-particle system.

IV. DEPLETION EFFECT

We recall that a constant N_0 enters into the effective Hamiltonian in Eq. (2.3), as a result of the replacement of a_0^* and a_0 by $(N_0)^{1/2}$ in the original Hamiltonian (2.1). Because of this approximation, the Hamiltonian no longer commutes with the number operator $\sum_{\mathbf{k}}a_{\mathbf{k}}^*a_{\mathbf{k}}$; in other words, the total number of particles is no longer conserved. However, to make the calculation self-consistent, we still have to relate N_0 to N, the total number of particles under the *same* approximation scheme. This is the aim of this section.

In Sec. II, we have diagonalized the effective Hamiltonian, H_{eff}, by a Bogoliubov transformation of the

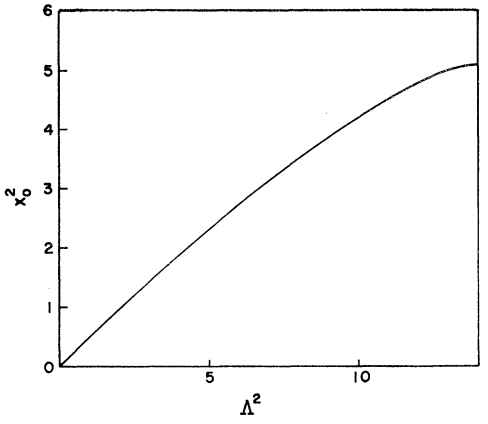

FIG. 2. Dependence of the interaction strength Λ^2 on the density x_0^2. The definitions for x_0^2 and Λ^2 can be found in the text. The screening factor D_0 can be obtained from $D_0=x_0^2/\Lambda^2$.

form of (2.5). This is equivalent to choosing the following right and left ground-state vectors of H_{eff}:

$$|\phi_0\rangle=\prod_{k>0} K_k \exp(-\alpha_k a_k {a^*}_k)|N\rangle$$
$$\langle\tilde{\phi}_0|=\prod_{k>0} \bar{K}_k\langle N|\exp(-\bar{\alpha}_k a_k a_{-k}), \tag{4.1}$$

where $|N\rangle$ is the N-free-particle ground-state vector related to the null-particle state vector $|0\rangle$ by

$$|N\rangle=(N!)^{-1/2}(a_0^*)^N|0\rangle, \tag{4.2}$$

and where K_k and $\bar{K}_k$ are normalization constants satisfying

$$K_k\bar{K}_k=1-\alpha_k\bar{\alpha}_k. \tag{4.3}$$

From (4.1) and (4.3) we obtain the expectation value,

$$\langle\tilde{\phi}_0|a_k^* a_k|\phi_0\rangle=\alpha_k\bar{\alpha}_k/(1-\alpha_k\bar{\alpha}_k). \tag{4.4}$$

If the whole system is in the ground state, we have

$$N-N_0=\lim_{\epsilon\to 0}\sum_{k\neq 0}\langle\tilde{\phi}_0|a_k^* a_k|\phi_0\rangle \tag{4.5}$$

Replacing the sum $\sum_k$ above by an integral, and then substituting (4.4) into (4.5), we obtain the following equation in terms of dimensionless quantities:

$$x_T^2-x_0^2=-\frac{4}{\pi}\lim_{\epsilon\to 0}\int_0^\infty dx\frac{x^2\alpha_x\bar{\alpha}_x}{1-\alpha_x\bar{\alpha}_x}, \tag{4.6}$$

where

$$x_T^2\equiv 8\pi a^3\rho, \tag{4.7}$$

with

$$\rho\equiv N/\Omega,$$

which is the true density of the system.

Since the T matrix is known from Sec. III, the two functions α_x and $\bar{\alpha}_x$ can be written out explicitly from Eqs. (2.6) and (2.8). In addition to T_k, which is given explicitly by (3.10), α_x and $\bar{\alpha}_x$ contain the following two T-matrix elements, which can be written out as follows:

$$T_{k-k,00}=(4\pi\hbar^2 a/m\Omega D_0)(\sin ka/ka),$$
$$T_{00,k-k}=(4\pi\hbar^2 a/m\Omega D_0)\cos k(a+\epsilon). \tag{4.8}$$

Using these forms for the T-matrix elements and after some straightforward manipulation, we can rewrite (4.6) as

$$x_T^2-x_0^2=\frac{2}{\pi}\int_0^\infty dx\, x^2[(1-A)^{-1/2}-1], \tag{4.9}$$

where

$$A=\Lambda^4(\sin 2x/2x)[x^2+\tfrac{1}{2}\Lambda^2(\sin x/x+\cos x)]^{-2}. \tag{4.10}$$

In Eq. (4.9) we have interchanged the limit $\epsilon\to 0$ and the integration, as a careful inspection of the integrand shows that this interchange is allowed.

The integral in (4.9) is calculated by numerical procedures for $\Lambda^2\lesssim 13$ and the results are shown in Fig. 3, which is a plot of x_0^2 versus Λ^2. We see that in general x_0^2 deviates very little from x_T^2 for a range of values of the screening factor. In other words, although the particles interact with each other, a very large fraction of them still remain at the zero-momentum state. Hence, the depletion effect is not important in the present calculation.

V. EXCITATION SPECTRUM OF LIQUID HELIUM II

We use the T-matrix elements of Eqs. (3.10) and (4.8) and obtain the excitation spectrum given by Eq. (2.11) as follows:

$$(2ma^2/\hbar^2)E_{ex}(x)=[x^4+\Lambda^2x^2(\sin x/x+\cos x)+\tfrac{1}{4}\Lambda^4(\cos x-\sin x/x)^2]^{1/2}. \tag{5.1}$$

Comparing this with Eq. (5.1) in Ref. 10, we see that the two excitation spectra are identical, except that the constant x_0^2 in Ref. 10 is now replaced by Λ^2. This is an expected result, since $x_0^2\equiv 8\pi a^3\rho_0$ is a dimensionless quantity which characterizes the interaction strength, and which must get modified when we have taken into account the structure of the interaction vertex in the T-matrix formalism. A plot of E_{ex} versus x given by Eq. (5.1) can be found in Fig. 1 of Ref. 10 with the replacement of x_0^2 by Λ^2, and it is not to be reproduced here.

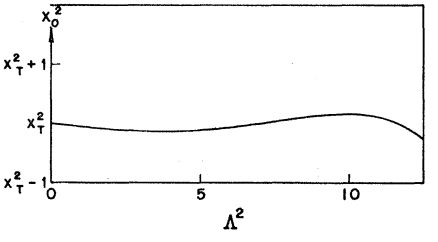

FIG. 3. Dependence of the depletion effect on the interaction strength. The definitions for x_T^2, x_0^2, and Λ^2 are contained in the text.

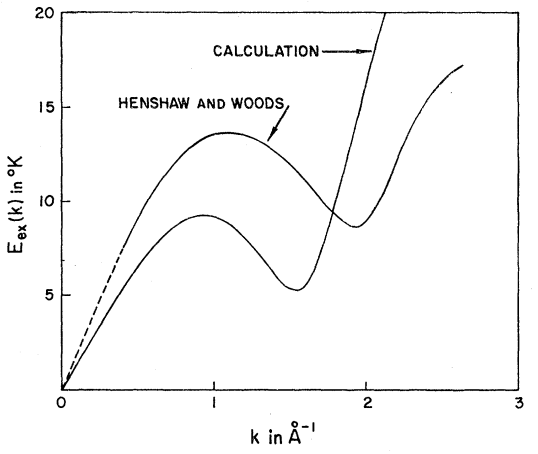

FIG. 4. Calculated excitation spectrum in liquid helium is compared with the experimental curve of Henshaw and Woods. The dashed portion of the curve represents extrapolation from the experimental data.

For liquid helium, the density ρ is equal to $(3.6\ \text{Å})^{-3}$ and the hard-core diameter a is taken as 2.1 Å. The choice of the value for a is consistent with the diameter of the repulsive core of about 2.5 Å in the Slater-Kirkwood[12] potential. For the chosen parameters, $x_T^2=5.0$. Then, by superimposing the two curves in Fig. 2 and in Fig. 3 (centered around $x_0^2=5.0$) together, we find the intersecting point at $\Lambda^2=12$ and $x_0^2=4.8$. Putting $\Lambda^2=12$ in Eq. (5.1) we obtain an excitation spectrum, which is shown in Fig. 4. In this figure we plot E_{ex} versus k in which E_{ex} is expressed in terms of degrees Kelvin, using the following conversion factor for helium:

$$\hbar^2/2ma^2=[6.06/a^2(\text{in Å}^2)]^\circ\text{K}.$$

The experimental curve of Henshaw and Woods[2] is also included in the same figure for comparison.

Although the agreement between the theoretical and experimental spectra is only qualitative, the theoretical spectrum does bend over to exhibit a roton-type dip.

VI. DISCUSSIONS

In this section we would like to discuss the following points: a comparison of the present method with that of B-S, the validity of the pseudopotential used, and the approximations made in the present paper and possible improvements.

In our calculations, we have worked with equations in momentum space all the way through. This is different from the procedures of B-S, who had to transform the T-matrix equation to the configuration space in order to handle the hard-sphere interaction. But, if this is the only difference, we should not have gotten a different excitation spectrum, and a different evaluation of the depletion effect.[9] Therefore, we examine more carefully and we see that the effective two-body interaction which B-S used in their calculation is a screened δ-function potential centered at $r=a$. In other words, their hard spheres are not really hard, but are capable of penetrating into each other. The error introduced by this effect has been found to be small in the fermion problem by Bethe and Goldstone,[13] but it is evidently not the case for a boson system.

Then, the question arises as to how good a replacement for hard-sphere interaction is our pseudopotential (3.1). As discussed in Ref. 10, it is an exact replacement of the hard-sphere boundary condition on the two-particle wave function except, however, for a discrete set of values of the relative momentum, with which the two hard spheres can still penetrate each other. Then, what would be the errors in our results caused by this effect? Our answer is that there would be none, and we give a brief argument in support of this view in the rest of this paragraph. Our pseudopotential is non-Hermitian and at the same time has this mentioned defect. To remove this defect we can construct an operator $\Delta(r)P$ defined as follows: $\Delta(r)$ is a step function,

$$\Delta(r)=0 \quad \text{if} \quad r>a,$$
$$=1 \quad \text{if} \quad r\leq a,$$

and P is a projection operator, which projects out the set of states with the particular momentum eigenvalues we mentioned before. Then, the exact pseudopotential for the two-body interaction should be given by our pseudopotential $V(r,\partial/\partial r)$ plus another term $(\hbar^2/2m)\times\nabla^2\Delta(r)P$. At the same time, this exact pseudopotential is hermitian. We refer to a paper by Wong[14] for discussions on this operator. But the important point is that the defect of our present pseudopotential is connected with its non-Hermiticity. As we have treated our non-Hermitian Hamiltonian by a procedure which involves taking its expectation value with respect to a right-state vector different from its left counterpart, the defect of our pseudopotential has been removed in this process. For example, if we use our pseudopotential and different right- and left-state vectors to calculate the pair distribution function in a straightforward manner, the calculated distribution function vanishes for $r\leq a$, as it should. Since the Fourier transform of the pair distribution function is connected with the excitation spectrum as described by Feynman,[3] a non-Hermitian pseudopotential which gives a good pair distribution function should also give a correct spectrum in the same framework.

As far as the calculation for the many-boson system is concerned, we have adopted several approximations in addition to only summing up selected terms in the per-

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turbation series. The validity of these approximations has already been mentioned in Sec. III except the following one: In the two particle Green's function (3.8), the two particles are assumed to be excited to the intermediate states from zero-momentum states. This approximation makes the screening factors D_l momentum-independent, and it seems to be a poor approximation especially for large momentum. However, its effect on the excitation spectrum can not be known until a numerical procedure is applied to find out the momentum dependence of D_l. This investigation is presently being carried out and the results will be reported separately.

In summary, we have derived an excitation spectrum in liquid helium in good qualitative agreement with experiments by assuming a hard-sphere-model potential. It is, therefore, hopeful that by taking a more realistic potential for helium including an attractive tail and by improving some of our calculational procedures, mainly the momentum dependence of the screening factors, we may even achieve a quantitative agreement between the spectrum calculated from first principles and that from experiments.

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Finite Superconductors and their Infinite Volume Limit*

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It is demonstrated that the standard applications of the BCS theory to finite systems does not possess the proper asymptotic behavior as the size of the system becomes infinite. In particular, no coupling exists from discrete states to those of positive energy unless the two-body potential is very strong (i.e., stronger than nuclear potentials). Two methods of correcting this deficiency are suggested: (a) a generalization of the BCS variational wave function, and (b) an extension of the Bogoliubov principle of compensating dangerous diagrams.

I. INTRODUCTION

With the introduction of phenomenological pairing interactions, the theory of superconductivity, as adapted to finite systems[1] is successful in explaining the spectra of low-lying states of many nuclei and the thermodynamic properties of finite metallic superconductors. We wish to point out that no coupling exists from discrete to continuum states in this theory, and consequently it does not approach the normal BCS[2] theory as the size of the system becomes infinite. We show, however, that this failure can be rectified to order $(\Delta/E_F)^2$ by either (a) a generalization of the BCS variational-type wave function, or (b) an extension of the Bogoliubov principle of compensating dangerous diagrams.

The BCS "integral" equation for the energy gap of a finite or infinite system is

$$\Delta_\alpha = -\tfrac{1}{2}\sum_{\alpha'} \frac{\langle \alpha - \alpha | V | \alpha' - \alpha' \rangle \Delta_{\alpha'}}{(\Delta_{\alpha'}^2 + \epsilon_{\alpha'}^2)^{1/2}}, \tag{1}$$

where $|-\alpha\rangle$ denotes the single-particle state time reversed with respect to the state $|\alpha\rangle$, and ϵ_α is the single-particle energy measured with respect to the Fermi energy E_F. For a finite system, the eigenstates we consider are those of fermions bound in a self-consistent single-particle potential well of dimension l. The energy spectrum consists of a discrete part, labeled by quantum numbers n, m and a continuum set labeled by indices k, l. Equation (1) can be separated as follows:

$$\Delta_n = -\tfrac{1}{2}\textstyle\sum_{n'} V_{nn'}\Delta_{n'}/E_{n'} - \frac{1}{2}\int_{k'} V_{nk'}\Delta_{k'}/E_{k'}, \tag{2a}$$

$$\Delta_k = -\tfrac{1}{2}\textstyle\sum_{n'} V_{kn'}\Delta_{n'}/E_{n'} - \frac{1}{2}\int_{k'} V_{kk'}\Delta_{k'}/E_{k'}, \tag{2b}$$

where $V_{\alpha\alpha'} = \langle \alpha - \alpha | V | \alpha' - \alpha' \rangle$ and $E_\alpha = (\Delta_\alpha^2 + \epsilon_\alpha^2)^{1/2}$. Here $\int_k \equiv \sum_k \to (L/2\pi)^3 \int d^3k$, where L is the dimen-

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