Equivalent wave-function approach to the ^{4}He structure factor and excitation spectrum

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A new method for the calculation of the excitation spectrum of liquid ^{4}He is developed based on the wave function $\chi_\alpha(x_1,x_2) = \langle 0|T\psi^\dagger(x_1)\psi(x_2)|\alpha\rangle$ that is directly related to and completely determines the dynamic structure factor $S(\vec{k},\omega)$ of liquid ^{4}He, and then employing this method a calculation of the sound spectrum of liquid ^{4}He is performed taking explicitly into account the depletion effect although it is based on the McMillan's data for the ground-state momentum distribution of liquid ^{4}He. First, by employing the exponential-decay and effective-mass approximation for the single-particle Green's function, the two-time Bethe-Salpeter integral equation for $\chi_\alpha(x_1,x_2)$ is transformed into the one-time Schrödinger equation. This is thus an approximate Schrödinger equation the solutions of which give $S(\vec{k},\omega)$ of liquid ^{4}He. In the exponential-decay approximation, the numerators of the single-particle Green's function are the true momentum distribution $N_{\vec{q}}$ of the ground state of liquid ^{4}He, which then enters into the Schrödinger equation in an essential way. Through this $N_{\vec{q}}$, both the presence of a condensate and the large depletion of particles from the zero-momentum state in ^{4}He can be properly taken into account. And the effective mass of a helium atom is determined using the McMillan's data and the Lennard-Jones potential. The Schrödinger equation is then solved in the limit $k\to 0$ using the McMillan's data, and an excitation spectrum of ^{4}He of the form $[\epsilon_k'^2 + 2\alpha n v(\vec{k})\epsilon_k'/(1+D)]^{1/2}$ in the limit $k\to 0$ is obtained, which differs from the Bogoliubov form by the factor $(1+D)^{-1}$ and the replacement of the bare mass m by the effective mass m^*. D, being proportional to $(1-\alpha)n$, represents the depletion effect. The expansion of the above expression gives for the sound velocity of liquid ^{4}He $c = 190$ m/sec and verifies the positive phonon dispersion.

I. INTRODUCTION

The excitation spectrum of liquid ^{4}He is just the singularities of the dynamic structure factor $S(\vec{k},\omega)$ of ^{4}He at $T=0$ °K, which is the Fourier transform of

$$S(x,x') \equiv \frac{1}{2\pi N}\langle\Psi_0|\psi^\dagger(x)\psi(x)\psi^\dagger(x')\psi(x')|\Psi_0\rangle , \quad (1.1)$$

where $x \equiv (\vec{x},t)$, $|\Psi_0\rangle$ denotes the ground state of the N-particle ^{4}He and we use the normalization $V=1$, where V is the volume. Let the completeness relation for $S(x,x')$ read as

$$\sum_{\vec{k},E} |\Psi_{\vec{k},E}\rangle\langle\Psi_{\vec{k},E}| = 1 , \quad (1.2)$$

where a state is labeled by total momentum $\vec{k}$, energy E (and other quantum number α; for simplicity, however, the index E will be understood to include the index α). $S(\vec{k},\omega)$ can then be written in the form

$$S(\vec{k},\omega) = \frac{1}{N}\sum_E \delta(\omega - (E-E_0))|\chi_{\vec{k},E}(0,0)|^2 , \quad (1.3)$$

where

$$\chi_{\vec{k},E}(x_1,x_2) \equiv \langle\Psi_0|T\psi^\dagger(x_1)\psi(x_2)|\Psi_{\vec{k},E}\rangle , \quad (1.4)$$

E_0 denotes the ground-state energy, and T the time-ordering operator. From this expression we see that $S(\vec{k},\omega)$ is directly related to and completely determined by the wave function $\chi_{\vec{k},E}(x_1,x_2)$. Therefore, the problem of determining $S(\vec{k},\omega)$ and the excitation spectrum of ^{4}He reduces to determining the wave function $\chi_{\vec{k},E}(x_1,x_2)$.

We also note that the ordinary t-matrix formalism is not concerned with this wave function. This is because, while the dynamic structure factor $S(x,x')$ is a particular case of the propagation $\langle\Psi_0|T\psi^\dagger(x_1)\psi(x_2)\psi^\dagger(x_4)\psi(x_3)|\Psi_0\rangle$ with $t_1,\ t_2 > t_3,\ t_4$ [which will be referred to as the $(\downarrow,\uparrow)$ propagation], the ordinary t-matrix formalism is associated with the propagation $\langle\Psi_0|T\psi(x_1)\psi(x_2)\psi^\dagger(x_4)\psi^\dagger(x_3)|\Psi_0\rangle$ with $t_1,\ t_2 > t_3,\ t_4$ [which will be referred to as the $(\uparrow,\uparrow)$ propagation].

There exist many calculations of the excitation spectrum of ^{4}He.[1] To the best of our knowledge, however, none of these takes explicitly into account, through the actual ground-state momentum distribution of ^{4}He, the effect of the (very large) depletion of particles from the zero-momentum state as a consequence of the strong helium interaction. It is obvious that taking explicitly into account the depletion effect through the ground-state momentum distribution is of decisive importance in the determination of the excitation spectrum.

Motivated by the above observations, we here attempt first to develop a new method for calculating the excitation spectrum of ^{4}He based on the wave function $\chi_{\vec{k},E}(x_1,x_2)$ that is, as shown above, directly related to and completely determines

$S(\vec{k}, \omega)$ (whereas the Brueckner-Sawada method[2] is based on the t-matrix which has been one of the major methods for calculating the excitation spectrum of ^{4}He) and then by employing this method to perform a calculation of the excitation spectrum of ^{4}He taking explicitly into account the depletion effect through the ground-state momentum distribution of ^{4}He, although it is based on the McMillan's data[3] for the ground-state momentum distribution.

We apply to the single-particle Green's function $\langle\Psi_0|a_{\vec{k}}(t)a_{\vec{k}}^\dagger|\Psi_0\rangle$ the exponential-decay law together with the effective-mass approximation for the energy denominator. With the use of this exponential-decay and effective-mass approximation for the single-particle Greens's function, we were able to transform the two-time Bethe-Salpeter integral equation for the wave function $\chi_{\vec{k},E}(x_1, x_2)$ into the one-time Schrödinger equation. This is thus an approximate Schrödinger equation the solutions of which give $S(\vec{k}, \omega)$. In the exponential-decay approximation, the numerators of the single-particle Green's function are the "true" momentum distribution $N_{\vec{q}}$ of the ground state of ^{4}He, which then enters into the Schrödinger equation in an essential way. Through this $N_{\vec{q}}$ both the presence of a condensate and the large depletion of particles from the zero-momentum state in ^{4}He can be properly taken into account. And the effective mass of a helium atom is determined using the McMillan's data and the Lennard-Jones potential. The Schrödinger equation is then solved in the limit $k \to 0$ (using McMillan's data) and the results as given in the abstract are obtained. In Sec. II, the Schrödinger equation is derived and the effective mass is determined. In Sec. III the Schrödinger equation is solved. Finally, in Sec. VI a discussion of the results is given.

II. DERIVATION OF THE SCHRÖDINGER EQUATION DETERMINING $S(\vec{k},\omega)$

A. Bethe-Salpeter equation

Separating the center-of-mass motion and in relative motion, the wave function $\chi_{\vec{k},E}(x_1, x_2)$ (1.4) can be written in the form

$$\chi_{\vec{k},E}(x_1, x_2) = e^{iK\cdot X}\chi'_{\vec{k},E}(x), \tag{2.1}$$

$$\chi'_{\vec{k},E}(x) \equiv \langle\Psi_0|T\psi^\dagger(\tfrac{1}{2}x)\psi(-\tfrac{1}{2}x)|\Psi_{\vec{k},E}\rangle, \tag{2.2}$$

where

$$K \equiv (\vec{k}, E - E_0), \quad X \equiv \tfrac{1}{2}(x_1 + x_2), \quad x \equiv x_1 - x_2, \tag{2.3}$$

and $a \cdot b$ denotes the usual scalar product of four-vectors a and b. Wave function $\chi'_{\vec{k},E}(x)$, when $t = 0$, becomes exactly the corresponding Schrödinger relative wave function

$$\phi'_{\vec{k},E}(\vec{x}) = \chi'_{\vec{k},E}(\vec{x}, t = 0)$$

$$= \langle\Psi_0|\psi^\dagger(\tfrac{1}{2}\vec{x}, 0)\psi(-\tfrac{1}{2}\vec{x}, 0)|\Psi_{\vec{k},E}\rangle \tag{2.4}$$

associated with the pair $(\downarrow,\uparrow)$ propagation. We shall hereafter omit the primes on χ' and ϕ'. We now introduce the equation for $\chi_{\vec{k},E}(x_1, x_2)$ usually known as the Bethe-Salpeter (BS) equation.[4] In general, the complete set of states in (1.2) is, for each $\vec{k}$, composed of discrete elements plus continuous elements. The former are the solutions to the homogeneous integral equation while the latter the inhomogeneous integral equation. But this paper is concerned only with the discrete elements. We also approximate the interaction kernel associated with the $(\downarrow, \uparrow)$ propagation, as usual, by the annihilation interaction plus the direct interaction in lowest order.[5,6] Our BS equation in momentum space is then

$$\chi_{\vec{k},E}(q) = [G(q + \tfrac{1}{2}K)G(q - \tfrac{1}{2}K)] \times \frac{1}{2\pi}\int dq' \,[iv(\vec{k}) + iv(\vec{q} - \vec{q}')]\chi_{\vec{k},E}(q'), \tag{2.5}$$

where $q \equiv (\vec{q}, \omega)$, dq denotes the four-volume element, $v(\vec{q})$, $\chi_{\vec{k},E}(q)$ and $G(q)$ are Fourier transforms of the interparticle potential $v(\vec{x})$, $\chi_{\vec{k},E}(x)$, and the single-particle Green's function

$$G(x_1, x_2) \equiv (-i)^2\langle\Psi_0|T\psi(x_1)\psi^\dagger(x_2)|\Psi_0\rangle, \tag{2.6}$$

respectively. In (2.5), the first term arises from the annihilation interaction and the second term the direct interaction. Equation (2.5) is the starting equation for our theory. In terms of the Schrödinger wave function in momentum space defined by

$$\phi_{\vec{k},E}(\vec{q}) = \int d^3x\, e^{-i\vec{q}\cdot\vec{x}}\phi_{\vec{k},E}(\vec{x}) = \frac{1}{2\pi}\int d\omega\, \chi_{\vec{k},E}(q), \quad q = (\vec{q}, \omega), \tag{2.7}$$

the BS equation (2.5) further becomes

$$\phi_{\vec{k},E}(\vec{q}) = \frac{i}{2\pi}\int d\omega\, G(q + \tfrac{1}{2}K)G(q - \tfrac{1}{2}K) \times \sum_{\vec{q}'}[v(\vec{k}) + v(\vec{q} - \vec{q}')]\phi_{\vec{k},E}(\vec{q}'). \tag{2.8}$$

B. Exponential-decay and effective-mass approximation for the single-particle Green's function

The BS equation (2.5) contains the single-particle Green's functions G and hence in order to do any

calculations we first have to choose an approximation for G. The single-particle Green's function in momentum space is given by

$$\begin{aligned} &G(\vec{k},t)=G_+(\vec{k},t)+G_-(\vec{k},t)\ , \\ &G_+(\vec{k},t)\equiv -i\Theta(t)\langle\Psi_0|a_{\vec{k}}(t)a_{\vec{k}}^\dagger|\Psi_0\rangle\ , \\ &G_-(\vec{k},t)\equiv -i\Theta(-t)\langle\Psi_0|a_{\vec{k}}^\dagger a_{\vec{k}}(t)|\Psi_0\rangle\ . \end{aligned} \tag{2.9}$$

(We here consider only the boson systems.) The amplitude $\exp(-iE_0t)\langle\Psi_0|a_{\vec{k}}(t)a_{\vec{k}}^\dagger|\Psi_0\rangle$, apart from a multiplicative constant, represents precisely the probability amplitude that the system will remain in its initial state at a later time $t>0$ when an extra particle of momentum $\vec{k}$ is added at $t=0$.[7] We apply to this amplitude the exponential decay law which has been widely used in physics. Our amplitude $\langle\Psi_0|a_{\vec{k}}(t)a_{\vec{k}}^\dagger|\Psi_0\rangle$ will then have the form

$$\begin{aligned} \langle\Psi_0|a_{\vec{k}}(t)a_{\vec{k}}^\dagger|\Psi_0\rangle &= \langle\Psi_0|a_{\vec{k}}a_{\vec{k}}^\dagger|\Psi_0\rangle \\ &\times\exp(-i\bar{\epsilon}_{\vec{k},+}t-\tfrac{1}{2}\Gamma_{\vec{k},+}t)\ ,\quad t\geq 0\ , \end{aligned} \tag{2.10}$$

where $\bar{\epsilon}_{\vec{k},+}$ denotes some real number and $\Gamma_{\vec{k},+}$ denotes the decay rate constant. The exponential-decay approximation for the single-particle Green's function is then

$$G_+(\vec{k},t)=-i(1+N_{\vec{k}})\exp(-iE_{\vec{k},+}t),\quad t\geq 0\ , \tag{2.11}$$

$$G_+(\vec{k},\omega)=(1+N_{\vec{k}})/(\omega-E_{\vec{k},+})\ , \tag{2.12}$$

where

$$N_{\vec{k}}\equiv\langle\Psi_0|a_{\vec{k}}^\dagger a_{\vec{k}}|\Psi_0\rangle\ , \tag{2.13}$$

$$E_{\vec{k},+}\equiv\bar{\epsilon}_{\vec{k},+}-\tfrac{1}{2}i\Gamma_{\vec{k},+},\quad \mathrm{Im}E_{\vec{k},+}\leq 0\ , \tag{2.14}$$

and similarly,

$$G_-(\vec{k},t)=-iN_{\vec{k}}\exp(-iE_{\vec{k},-}t),\quad t\leq 0\ , \tag{2.15}$$

$$G_-(\vec{k},\omega)=-N_{\vec{k}}/(\omega-E_{\vec{k},-})\ , \tag{2.16}$$

where

$$E_{\vec{k},-}\equiv\bar{\epsilon}_{\vec{k},-}+\tfrac{1}{2}i\Gamma_{\vec{k},-},\quad \mathrm{Im}E_{\vec{k},-}\geq 0\ . \tag{2.17}$$

Further, the two propagations described by $G_\pm(\vec{k},t)$ are precisely the time-reversed conjugate of each other and then invariance under time reversal implies that[8]

$$\begin{aligned} &\mathrm{Re}E_{\vec{k},+}=\mathrm{Re}E_{\vec{k},-}\ , \\ &\mathrm{Im}E_{\vec{k},+}=-\mathrm{Im}E_{\vec{k},-}\ . \end{aligned} \tag{2.18}$$

For the energy denominator $E_{\vec{k},+}$, we choose the single-particle energy in accordance with the Brueckner-Sawada theory; in the Brueckner-Sawada method, the single-particle energy is chosen for the energy denominator of the propagator in the t-matrix equation.[9] Further, it is customary to approximate the momentum dependence of the single-particle energy by a quadratic function, which gives rise to the concept of the effective mass m^*. Thus, in such an effective-mass approximation, we have

$$E_{\vec{k},+}=\epsilon'_{\vec{k}}+\nu-i\epsilon\ , \tag{2.19}$$

where $\epsilon'_{\vec{k}}\equiv k^2/2m^*$, ν is a constant, and $\epsilon\to 0+$.

The exponential-decay and effective-mass approximation for the single-particle Green's function is then

$$G(\vec{k},\omega)=\frac{1+N_{\vec{k}}}{\omega-\epsilon'_{\vec{k}}-\nu+i\epsilon}-\frac{N_{\vec{k}}}{\omega-\epsilon'_{\vec{k}}-\nu-i\epsilon}\ . \tag{2.20}$$

It should be noted that $N_{\vec{k}}$, being given by (2.13), is the "true" momentum distribution of the ground state of the system and therefore the existence of a condensate in ^{4}He poses no additional difficulties, since it will be properly taken into account through th $N_{\vec{k}}$. Some justification for employing the simple effective-mass approximation in the single-particle Green's functions in the BS equation will be made at the end of the present section.

We now turn to the determination of the effective mass of a helium atom. A simple approximation for the single-particle potential $U(\vec{k})$ in a system with a hard-core potential can be obtained quite simply by inserting a cutoff into the Hartree-Fock single-particle self-energy and, in addition, by replacing the Hartree-Fock momentum distribution by the true momentum distribution. This cutoff of course arises from the fact that the particles can never penetrate each other's hard cores. We thus have

$$U(\vec{k})=n\int_{|\vec{x}|>r_0}d^3x\,v(\vec{x})+\int_{|\vec{x}|>r_0}d^3x\,\rho_1(\vec{x})v(\vec{x})e^{-i\vec{k}\cdot\vec{x}}\ , \tag{2.21}$$

where n denotes the particle density, r_0 is the hard-core radius, and $\rho_1(\vec{x})$ the true single-particle density matrix of the ground state defined by

$$\rho_1(\vec{x})=\sum_{\vec{q}}e^{i\vec{q}\cdot\vec{x}}N_{\vec{q}}\ . \tag{2.22}$$

The effective mass defined by $m^*=m(1+2mb/\hbar^2)^{-1}$ with the expansion $U(\vec{k})\approx U(0)+bk^2$ is then

$$m^*=m\left(1-\frac{4\pi m}{3\hbar^2}\int_{r>r_0}dr\,r^4\rho_1(r)v(r)\right)^{-1}\ . \tag{2.23}$$

This integration was carried out numerically for three different values of the hard-core radius, $r_0=2.3$, 2.556, 2.8 Å, up to $r_\infty=10\,200$ Å (instead of $r_\infty=\infty$), by using the Lennard-Jones potential and

TABLE I. Effective mass of a helium atom for three hard-core radii.

r_0 (Å)	m^*/m
2.3	0.241 147 93
2.556	0.217 283 68
2.8	0.224 762 76

the following Gaussian fit[10] to the McMillan data for the momentum distribution or the single-particle density matrix of the ground state of ^{4}He:

$$\rho_1(r) = \alpha n + (1-\alpha) n e^{-r^2/2a^2} , \tag{2.24}$$

where the condensate fraction $\alpha = 0.11$, $n = 2.20 \times 10^{-2}$ atoms/Å^3, and $a = 1.35$ Å. Results are given in Table I. They exhibit a surprisingly remarkable feature: they are not sensitive to changes in the hard-core radius about the value $r_0 = \sigma = 2.556$ Å. Therefore σ may be taken to be the hard-core radius r_0 and then from Table I,

$$m^* \approx 0.217 m . \tag{2.25}$$

It can be easily shown that the error made in replacing the upper limit $r_\infty = \infty$ by $r_\infty = 10\,200$ Å (for the case $r_0 = \sigma$) is less than 0.03%.

C. Schrödinger equation determining $S(\vec{k},\omega)$

For practical solution, it is convenient if the integral equation (2.8) can be transformed into a differential equation (just as the ordinary t-matrix integral equation is transformed into a differential equation, the Bethe-Goldstone equation[11]). This is possible by use of the exponential-decay and effective-mass approximation for the single-particle Green's function (2.20). Employing that approximation, it is easy to show that

$$\frac{i}{2\pi}\int d\omega\,[G(q+\tfrac{1}{2}K)G(q-\tfrac{1}{2}K)]$$

$$= \frac{(1+N_{\vec{q}+\frac{1}{2}\vec{k}})N_{\vec{q}-\frac{1}{2}\vec{k}}}{E - E_0 - (\epsilon'_{\vec{q}+\frac{1}{2}\vec{k}} - \epsilon'_{\vec{q}-\frac{1}{2}\vec{k}}) + i\epsilon}$$

$$- \frac{N_{\vec{q}+\frac{1}{2}\vec{k}}(1+N_{\vec{q}-\frac{1}{2}\vec{k}})}{E - E_0 - (\epsilon'_{\vec{q}+\frac{1}{2}\vec{k}} - \epsilon'_{\vec{q}-\frac{1}{2}\vec{k}}) - i\epsilon} . \tag{2.26}$$

A useful formula here is, for any real X,[12]

$$X/X \pm i\epsilon = 1 . \tag{2.27}$$

Proof:

$$\frac{X}{X \pm i\epsilon} = 1 + \frac{\mp i\epsilon}{X \pm i\epsilon} = 1 + I, \quad I \equiv \frac{\mp i\epsilon}{X \pm i\epsilon} ,$$

$$|I|^2 = \pi\epsilon\delta(X) .$$

But, since $\epsilon \to 0$, we have $|I|^2 = I = 0$, Q.E.D. Applying this formula to (2.8) and (2.26), we obtain

$$(E - E_0 - \epsilon'_{\vec{q}+\frac{1}{2}\vec{k}} + \epsilon'_{\vec{q}-\frac{1}{2}\vec{k}})\phi_{\vec{k},E}(\vec{q}) = [(1+N_{\vec{q}+\frac{1}{2}\vec{k}})N_{\vec{q}-\frac{1}{2}\vec{k}} - N_{\vec{q}+\frac{1}{2}\vec{k}}(1+N_{\vec{q}-\frac{1}{2}\vec{k}})]\sum_{\vec{q}'}[v(\vec{k}) + v(\vec{q}-\vec{q}')]\phi_{\vec{k},E}(\vec{q}')$$

$$= (N_{\vec{q}-\frac{1}{2}\vec{k}} - N_{\vec{q}+\frac{1}{2}\vec{k}})\sum_{\vec{q}'}[v(\vec{k}) + v(\vec{q}-\vec{q}')]\,\phi_{\vec{k},E}(\vec{q}') . \tag{2.28}$$

In other words, when (2.8) with (2.26) is transformed into the corresponding differential equation, a difference in the boundary condition ($\pm i\epsilon$) no longer comes into effect and the two residues $(1+N)N\sum[v+v]$ and $-N(1+N)\sum[v+v]$ are summed algebraically. Physically, the former represents the effective interaction kernel associated with the $(\uparrow,\downarrow)$ propagation in the intermediate state while the latter the $(\downarrow,\uparrow)$ propagation. Then, the total interaction kernel that appears in the corresponding Schrödinger equation should be their algebraic sum. In configuration space, the above equation becomes ($\vec{k}$ here denotes momentum rather than wave number)

$$\left(E - E_0 + \frac{i\hbar}{m^*}\vec{k}\cdot\nabla\right)\phi_{\vec{k},E}(\vec{x})$$

$$= 2i\int d^3x'\,\sin\left(\frac{\vec{k}\cdot(\vec{x}-\vec{x}')}{2\hbar}\right)\rho_1(\vec{x}-\vec{x}')$$

$$\times[v(\vec{k})\delta(\vec{x}') + v(\vec{x}')]\phi_{\vec{k},E}(\vec{x}') . \tag{2.29}$$

Note that ν, a constant displacement in the energy denominator (2.19), does not enter into the equation as is evident from (2.26). Expression (1.3) can also be written in the form

$$S(\vec{k},\omega)=\frac{1}{N}\sum_{E}\delta(\omega-(E-E_0))\left|\phi_{\vec{k},E}(0)\right|^2 . \qquad (2.30)$$

(i) Result (2.29) is an approximate Schrödinger equation, the solutions of which give, through expression (2.30), the discrete part (i.e., the phonon-roton spectrum) of the dynamic structure factor $S(\vec{k},\omega)$ of ^{4}He.[13]

(ii) We have chosen, based on the exponential-decay law, the "true" momentum distribution $N_{\vec{q}}$ of the ground state for the numerators of the single-particle Green's functions in the BS equation. As a result, the $N_{\vec{q}}$ or the true single-particle density matrix $\rho_1(\vec{x})$ of the ground state enters, in an essential way, into the Schrödinger equation determining $S(\vec{k},\omega)$. This is in accord with our earlier observation that a proper consideration of the distribution of particles in the ground state should be of decisive importance in the determination of the excitation spectrum of ^{4}He. Through this $\rho_1(\vec{x})$, both the existence of the condensate and the (very large) depletion of particles from the zero-momentum state as a consequence of the strong helium interaction, can be taken explicitly into account.

(iii) We have chosen the effective-mass approximation (2.19) for the energy denominators of the single-particle Green's function, which corresponds only to an independent particle model and may be valid only for high k. As will be seen below, however, even the bare-pole approximation $E_{\vec{k},+}\approx\epsilon_{\vec{k}}-i\epsilon$ where $\epsilon_{\vec{k}}\equiv k^2/2m$ which completely ignores the effect of the interactions, already leads to a random-phase approximation (RPA) when employed in the single-particle Green's functions in the BS integral equation (by some authors, RPA has previously been applied[1,14] to ^{4}He). This, in some degree, justifies employing such simple effective-mass approximation in the single-particle Green's function in the BS integral equation. The effective-mass approximation leads to an improved form of RPA which differs from RPA by a replacement of the bare mass m by the effective mass m^* (approximately equal to the mass of an atom *inside* the medium).

(iv) It is easy to show that, if only the annihilation interaction term is retained, the Schrödinger equation (2.29) becomes the RPA dispersion relation (apart from the replacement of m by m^*).

III. SOLUTION IN THE LIMIT $k\to 0$

We now wish to solve the Schrödinger equation (2.29). The two basic interactions associated with the $(\downarrow,\uparrow)$ propagation are the annihilation interaction $v(\vec{k})\delta(\vec{x})$ and the direct interaction $v(\vec{x})$ as Eq. (28) of Ref. 6 indicates. These two interactions compete with each other. For helium potential, in the limit $k\to 0$, the annihilation interaction is much more important than the direct interaction, whereas as k increases, the direct interaction is equally important and even much more important than the annihilation interaction for sufficiently high k; the relative importance of these two interactions may be inferred from the factor on the right-hand side of (2.8):

$$\sum_{\vec{q}'}[v(\vec{k})+v(\vec{q}-\vec{q}')]\phi_{\vec{k},E}(\vec{q}') , \qquad (3.1)$$

where the first term arises from the annihilation interaction and the second term the direct interaction. The recent numerical calculations[15] indicate that Fourier transform of helium potential (i) should have a very large (infinite) maximum at $k=0$ (which is obvious), and (ii) should decrease monotonically with increasing k. It is then evident that in (3.1), in the limit $k\to 0$, the annihilation interaction term is much more important than the direct interaction term. (The same argument has been used for other cases.[5]) As k increases, however, because of (ii), the direct interaction term will be equally important. Further, for sufficiently high k, it will even be much more important than the annihilation interaction term.

The limit $k\to 0$ is the main objective of this work, however, so we retain only the annihilation term and the Schrödinger equation (2.29) becomes

$$\left(\omega+\frac{i\hbar}{m^*}\vec{k}\cdot\nabla\right)\phi_{\vec{k}}(\vec{x})\underset{k\to 0}{\cong}2iv(\vec{k})\phi_{\vec{k}}(0)\times\sin\left(\frac{\vec{k}\cdot\vec{x}}{2\hbar}\right)\rho_1(\vec{x}) , \qquad (3.2)$$

with $\omega\equiv E-E_0$, where we have omitted the index E on the wave function because it turns out that this equation possesses only one solution for each $\vec{k}$. Taking $\vec{k}=k\hat{x}$ $[\vec{x}=(x,y,z)]$ and using an integrating factor $e^{-i(m^*\omega/\hbar k)x}$, (3.2) can easily be transformed to

$$e^{-i(m^*\omega/\hbar k)x}\phi_{\vec{k}}(\vec{x})\underset{k\to 0}{=}-i\frac{m^*}{\hbar k}v(\vec{k})\phi_{\vec{k}}(0)\times\int^x dx\,(e^{-i(m^*/\hbar k)(\omega-\epsilon_{\vec{k}})x}-e^{-i(m^*/\hbar k)(\omega+\epsilon_{\vec{k}})x})\rho_1(\vec{x})+\text{const} , \qquad (3.3)$$

where $\int^x dx$ indicates an indefinite integral. But for ω to be an "eigenvalue," the constant must vanish and then (3.3) can be integrated by inserting (2.24) for $\rho_1(\vec{x})$:

$$\phi_{\vec{k}}(\vec{x}) \underset{k\to 0}{=} v(\vec{k})\phi_{\vec{k}}(0)\left\{\alpha n\left(\frac{e^{i(k/2\hbar)x}}{\omega-\epsilon'_{\vec{k}}}-\frac{e^{-i(k/2\hbar)x}}{\omega+\epsilon'_{\vec{k}}}\right)-i\frac{m^*}{\hbar k}(1-\alpha)n\sqrt{\tfrac{1}{2}\pi}\,a e^{i(m^*\omega/\hbar k)x-(y^2+z^2)/2a^2}\right.$$
$$\times\left[e^{-[(am^*/\sqrt{2}\,\hbar k)(\omega-\epsilon'_{\vec{k}})]^2}\operatorname{erf}\left(\frac{x}{\sqrt{2}\,a}+i\frac{am^*}{\sqrt{2}\,\hbar k}(\omega-\epsilon'_{\vec{k}})\right)\right.$$
$$\left.\left.-e^{-[(am^*/\sqrt{2}\,\hbar k)(\omega+\epsilon'_{\vec{k}})]^2}\operatorname{erf}\left(\frac{x}{\sqrt{2}\,a}+i\frac{am^*}{\sqrt{2}\,\hbar k}(\omega+\epsilon'_{\vec{k}})\right)\right]\right\},\quad \vec{k}=k\hat{x} \tag{3.4}$$

where we have used the relation

$$\int^x dt\, e^{-t^2/2a^2-ibt}$$
$$=\sqrt{\tfrac{1}{2}\pi}\,a e^{-(ab/\sqrt{2})^2}\operatorname{erf}\left(\frac{x}{\sqrt{2}\,a}+i\frac{ab}{\sqrt{2}}\right)\ , \tag{3.5}$$

with the error function $\operatorname{erf}t\equiv(2/\sqrt{\pi})\int_0^t dt\, e^{-t^2}$. To find the eigenvalue we put $\vec{x}=0$ in (3.4) and then we obtain the eigenvalue equation

$$\frac{1}{v(\vec{k})}\underset{k\to 0}{=}\alpha n\frac{2\epsilon'_{\vec{k}}}{\omega^2-\epsilon'^2_{\vec{k}}}+(1-\alpha)n\frac{\sqrt{2}\,am^*}{\hbar k}$$
$$\times\left[F\left(\frac{am^*}{\sqrt{2}\,\hbar k}(\omega-\epsilon'_{\vec{k}})\right)\right.$$
$$\left.-F\left(\frac{am^*}{\sqrt{2}\,\hbar k}(\omega+\epsilon'_{\vec{k}})\right)\right], \tag{3.6}$$

where $F(t)$ is defined by

$$F(t)\equiv i\tfrac{1}{2}\sqrt{\pi}\ e^{-t^2}\operatorname{erf}(it)=e^{-t^2}\int_0^t dt\, e^{t^2}\ . \tag{3.7}$$

We now use the self-consistency method to solve this eigenvalue equation. $F(t)$ has the following behavior[16]:

$$F(t)\approx t,\quad \text{for}\ \ 0\leq t\lesssim 0.2\ . \tag{3.8}$$

As will be seen below,

$$F\left(\frac{am^*}{\sqrt{2}\,\hbar k}(\omega\mp\epsilon'_{\vec{k}})\right)\underset{k\to 0}{=}\frac{am^*}{\sqrt{2}\,\hbar k}(\omega\mp\epsilon'_{\vec{k}}) \tag{3.9}$$

leads to the following solution of the eigenvalue equation:

$$\omega\underset{k\to 0}{\approx}ck\quad \text{with}\ c=\sqrt{\alpha}\ /\sqrt{1-\alpha}\,(\hbar/am^*)\ ,$$

which in turn permits the above relation (3.9) since it satisfies the condition in (3.8) that the argument should not exceed ≈ 0.2; with $\alpha=0.11$,

$$(am^*/\sqrt{2}\,\hbar k)(\omega\mp\epsilon'_{\vec{k}})\underset{k\to 0}{\approx}(am^*/\sqrt{2}\,\hbar k)ck$$
$$=(1/\sqrt{2}\,)\sqrt{\alpha}\ /\sqrt{1-\alpha}=0.25\ , \tag{3.10}$$

more precisely, we are here making the approximation

$$F(0.25)\approx 0.25\ , \tag{3.11}$$

whereas[16]

$$F(0.25)=0.24\ . \tag{3.12}$$

Note that the argument in (3.10) is actually dependent *only* on α. Then (3.6) becomes

$$\frac{1}{v(\vec{k})}\underset{k\to 0}{=}\alpha n\frac{2\epsilon'_{\vec{k}}}{\omega^2-\epsilon'^2_{\vec{k}}}+(1-\alpha)n\frac{\sqrt{2}\,am^*}{\hbar k}$$
$$\times\left(\frac{am^*}{\sqrt{2}\,\hbar k}(\omega-\epsilon'_{\vec{k}})-\frac{am^*}{\sqrt{2}\,\hbar k}(\omega+\epsilon'_{\vec{k}})\right)\ . \tag{3.13}$$

A somewhat different derivation of this relation is given in the Appendix. This relation gives (if $\alpha\neq 0$),

$$\omega\underset{k\to 0}{=}\left(\frac{2\alpha n v(\vec{k})}{1+D}\epsilon'_{\vec{k}}+\epsilon'^2_{\vec{k}}\right)^{1/2}, \tag{3.14}$$

where

$$D\equiv(1-\alpha)na^2\hbar^{-2}m^*v(\vec{k}),\quad k\to 0\ . \tag{3.15}$$

Since $v(\vec{k}\to 0)\to\infty$, it follows that

$$D\gg 1\ , \tag{3.16}$$

and thus finally have

$$\omega\underset{k\to 0}{=}\left(\frac{2\alpha n v(\vec{k})}{D}\epsilon'_{\vec{k}}+\epsilon'^2_{\vec{k}}\right)^{1/2}$$
$$=\left[\frac{\alpha}{1-\alpha}\left(\frac{\hbar}{am^*}\right)^2k^2+\frac{1}{4m^{*2}}k^4\right]^{1/2}$$
$$=ck(1+\gamma k^2)\ , \tag{3.17}$$

with

$$c=\left(\frac{\alpha}{1-\alpha}\right)^{1/2}\frac{\hbar}{am^*}\ ,\quad \gamma=\frac{1-\alpha}{\alpha}\frac{a^2}{8\hbar^2}\ . \tag{3.18}$$

When McMillan's results [$\alpha=0.11$ and $a=1.35$ Å, see (2.24)] and our calculated effective mass [$m^*=0.217$m, see (2.25)] are inserted, (3.18) gives

$$c=190\ \text{m sec}^{-1}$$
$$\gamma=16.6\times 10^{37}\,\text{g}^{-2}\,\text{cm}^{-2}\,\text{sec}^2,\ \text{at}\ T=0\,^\circ\text{K}\ , \tag{3.19}$$

to be compared with the experimental values[17]

$$c = 238 \text{ m sec}^{-1}$$
$$\gamma = 8 \sim 15 \times 10^{37} \text{ g}^{-2} \text{cm}^{-2} \text{sec}^2, \text{ at } T \simeq 0.3\,^{\circ}\text{K} . \tag{3.20}$$

IV. DISCUSSION

(i) D given by (3.15) being proportional to $(1-\alpha)n$ represents the depletion effect. (ii) Our result (3.17) verifies the positive phonon dispersion of ^{4}He proposed only recently.[18] (iii) With the value $\alpha = 0.11 \neq 0$ the first term of the eigenvalue equation (3.6) does not vanish. The form of the spectrum (3.17) in which the sound velocity is proportional to the condensate fraction comes from this first term, as can be seen from (3.6). Suppose we now consider the case that the interaction is so strong that there is no condensate, i.e., $\alpha = 0$. In that case (assuming the momentum distribution remains a Gaussian with different values of a and m^*), this first term disappears, which means that, for the case $\alpha = 0$, the spectrum is determined from an entirely different eigenvalue equation as compared with the case $\alpha \neq 0$. Therefore, one cannot argue, based on the extension of the result (3.17) to the limit $\alpha = 0$, that a spectrum of that type gives an unsatisfactory result that the sound spectrum cannot exist without condensate. (iv) The result (3.17) is obtained by taking into account only the annihilation interaction and ignoring the direct interaction which may be permitted only in the limit $k \to 0$ as already pointed out. This means that the spectrum (3.17) or a spectrum of Bogoliubov type [with $D = 0$ (3.14) becomes the Bogoliubov type] is valid only in the limit $k = 0$ so that the term $\epsilon_{\vec{k}}'^2$ serves only as a perturbation to the other term, with $v(\vec{k}) \approx v(0)$ as $k \to 0$. (v) For finite k, the direct interaction may no longer be ignored. We thus call attention to the importance of the direct interaction for finite k which has been ignored in obtaining a spectrum of Bogoliubov type. (vi) For high k, the direct interaction even dominates the dynamics. Let k_d be the onset momentum of the dominance of the direct interaction. For $k \geq k_d$, the Schrödinger equation to solve is thus

$$\left(\omega + \frac{i\hbar}{m^*}\vec{k}\cdot\nabla\right)\phi_{\vec{k}}(\vec{x}) \cong 2i \int d^3x' \sin\left(\frac{\vec{k}\cdot(\vec{x}-\vec{x}')}{2\hbar}\right) \times \rho_1(\vec{x}-\vec{x}')v(\vec{x}')\phi_{\vec{k}}(\vec{x}'), \quad k \geq k_d . \tag{4.1}$$

Using the same technique as in the case $k \to 0$ and taking into account only the condensate [i.e., with $\rho_1(\vec{x}) \approx \alpha n$)], it is easy to show that this equation gives

$$\omega \cong \{[\epsilon_{\vec{k}}' + \alpha n v(0)]^2 - (\alpha n)^2 v(\vec{k})^2\}^{1/2} \approx \epsilon_{\vec{k}}' + \alpha n v(0), \quad k \geq k_d \tag{4.2}$$

since $v(0) \gg v(\vec{k})$ for high k. This spectrum exhibits the essential features of the roton spectrum: there occurs a gap and the spectrum is quadratic in k. The Bogoliubov spectrum reduces to the form const$k$ as $k \to 0$ and hence provides a model for the phonon spectrum of ^{4}He. Similarly, there is a possibility that the spectrum (4.2) may also be a primitive form of the roton spectrum. The speculation is then that $k_r = k_d$, i.e., the roton minimum corresponds to the onset of the dominance of the direct interaction (whereas the annihilation interaction is most important in the limit $k \to 0$). In other words, while phonons arise primarily from the repeated annihilation interactions or RPA, there is a possibility that rotons may arise primarily from the repeated direct interactions or ladder diagrams associated with the $(\downarrow,\downarrow)$ [not $(\uparrow,\uparrow)$] propagation.

APPENDIX

If the solution ω is of the form

$$\omega \underset{k\to 0}{=} ck(1+\gamma k^2), \quad \text{with } c = \left(\frac{\alpha}{1-\alpha}\right)^{1/2} \frac{\hbar}{am^*} , \tag{A1}$$

where γ is not specified, then the second term ($\equiv I$) in the eigenvalue equation (3.6) becomes

$$I = \text{const}(1/k)[F(\lambda - \mu k + \nu k^2) - F(\lambda + \mu k + \nu k^2)] , \tag{A2}$$

where

$$\text{const} \equiv (1-\alpha)n(\sqrt{2}\, am^*/\hbar)$$
$$\lambda \equiv \frac{1}{\sqrt{2}}\left(\frac{\alpha}{1-\alpha}\right)^{1/2} = 0.25, \quad \mu \equiv \frac{a}{2\sqrt{2}\,\hbar}, \quad \upsilon \equiv \gamma\lambda, \tag{A3}$$

and

$$F(\lambda \mp \mu k + \nu k^2) \underset{k\to 0}{=} F(\lambda) + (\mp \mu k + \nu k^2)F'(\lambda) + \cdots , \tag{A4}$$

where $F'(\lambda)$ denotes the first derivative of $F(\lambda)$ with respect to λ. If we use the approximation [see (3.8), (3.11) and (3.12)]

$$F'(\lambda) = F'(0.25) \approx 1 , \tag{A5}$$

then the I becomes in the limit $k \to 0$

$$I \underset{k\to 0}{=} \text{const}(-2\mu)F'(\lambda) \underset{k\to 0}{\approx} -(1-\alpha)n\, a^2 m^*/\hbar^2 , \tag{A6}$$

which is the same as the second term in (3.13). The important point is that, because of the k

present in the denominator of the I, one must keep the first two terms [rather than just the first term $F(\lambda)$] in the expansion of (A4). Keeping only the first term would make the I vanish and lead to an entirely incorrect result. Now, (A6) or (3.13) leads to the solution (3.17) and (3.18). Thus the solution ω is indeed of the form (A1) as we assumed.

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