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Lambda transition and Bose-Einstein condensation in liquid ^{4}He

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We present the theory describing Bose-Einstein condensation (BEC) and superfluidity in a liquid ^{4}He based on the concept that for some temperature interval, there exist metastable diatomic clusters or diatomic quasiparticles which are the bound states of two atoms of ^{4}He. It is shown that in liquid ^{4}He for the temperature region $1\ \mathrm{K} \leqslant T \leqslant T_\lambda$ diatomic quasiparticles macroscopically populate the ground state which leads to BEC in liquid ^{4}He. The approach yields the lambda temperature as $T_\lambda = 2.16$ K, which is in excellent agreement with the experimental lambda transition temperature $T_\lambda = 2.17$ K. The concept of diatomic quasiparticles also leads to superfluid and BEC fractions which are in good agreement with experimental data and Monte Carlo simulations for liquid ^{4}He. It is also shown that the condensate fraction for low temperature ($T \leqslant 0.5$ K) at saturated vapor pressure is $\rho_0/\rho = 7.22\%$, which is very close to the value $7.25 \pm 0.75\%$ obtained in recent measurements.

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I. INTRODUCTION

The similarity between liquid ^{4}He and an ideal Bose-Einstein gas was recognized by London. He assumed that the lambda transition in liquid ^{4}He is the analog for a phase transition in an ideal Bose gas at low temperature [1,2]. This idea is supported by estimation based on an equation for the critical temperature in an ideal Bose gas. Thereafter, Tisza suggested that the presence of the condensed particles can be described by a two-fluid hydrodynamics [3]. In this model, the "condensate" completely has no friction, while the rest behave like an ordinary liquid. However, Tisza's model did not appear to be completely self-consistent and quantitative.

Two-fluid quantitative hydrodynamics was subsequently developed by Landau [4]. However, in this paper, the idea of Bose-Einstein condensation (BEC) is not assumed. Landau has predicted the excitation spectrum of liquid He II which changes from the phonon behavior $\epsilon(p) = cp$ at small momenta to a "rotonlike" form at larger values of the momenta as $\epsilon(p) = \Delta + (p - p_0)^2/2\mu_R$. This phenomenological model was based mostly on experimental data and deep physical intuition. The modern understanding of superfluidity is based on the Onsager-Feynman quantization condition, which is also important for the two-fluid theory in liquid ^{4}He [5]. The excitation spectrum in liquid ^{4}He was measured in neutron scattering experiments with great accuracy by several groups, in particular by Henshaw and Woods [6]. This spectrum qualitatively agrees with Landau's phenomenological excitation spectrum.

The Bogoliubov analytical results [7] for elementary excitations in the Bose gas are very important for understanding the excitation spectrum in a phonon region. Nevertheless, the Bogoliubov theory can be applied only to dilute Bose systems. Feynman has found a relation between the energy spectrum of the elementary excitations and the structure factor [8,9] that verifies Landau's phenomenological dispersion relation. We note that Feynman's relation is correct only for small enough momenta when the excitations are phonons. In a rotonlike region, it is only an approximation of a real situation. Feynman has also proposed a model of the roton excitation as a localized vortex ring [5] with a characteristic size of the order of a mean atomic distance in liquid ^{4}He. A number of methods have also been suggested for applications to quantum Bose liquids. For a review of quantum fluid theories, also see Refs. [10–21]. In the past few years, ultracold atomic systems have opened up the possibility to explore the concept of universality [22]. It manifests itself in that different physical systems can exhibit the same behavior, even if the relevant energy and length scale differ by many order of magnitude. These works have stimulated new experiments in ultracold Bose gases near a Feshbach resonance [23].

The use of neutrons to observe the condensate fraction in liquid ^{4}He was proposed in Refs. [24,25] and the first measurement of BEC fraction in liquid ^{4}He was reported by Cowley and Woods [26]. The history of measurement to higher incidence energy neutrons and improved spectrometer performance is reviewed by Glyde [27], Sokol [28], and others. The recent measurements of BEC and the atomic momentum distribution in liquid and solid ^{4}He are reported by Diallo, Glyde, and others [29–32]. The momentum distribution of liquid ^{4}He and ^{3}He has been calculated, at zero temperature, by using the Green-function Monte Carlo method [33] and the diffusion Monte Carlo method [34,35]. At finite temperature, the simulations have been done by the path-integral Monte Carlo method [36,37]. For bosons, they provide energy estimates that are virtually exact, within statistical accuracy. The optimization procedure based on Monte Carlo calculations has been proposed in Ref. [38].

Initiated by Wilson, the field-theoretical approach to critical phenomena has been extremely successful in the domain of a phase transition [39]. In particular, this theory describes the lambda transition in liquid ^{4}He. It has been possible to calculate the critical exponents through the Wilson-Fisher $\epsilon = 4 - d$ expansion [40]. The critical exponents can also be calculated in three dimensions from field theory [41]. The above-mentioned results provide the conceptual basis for the understanding of a lambda transition, superfluidity, and BEC in liquid ^{4}He. However, there are fundamental questions that are still open in this area. For example, there is no analytic quantitative theory describing the BEC and superfluid fractions in liquid ^{4}He below the lambda transition temperature T_λ.

In this paper, we develop the theory for superfluid ^{4}He based on the concept that for some temperature interval, there exist metastable diatomic clusters or diatomic quasiparticles (DQs) which are the bound states of two atoms of ^{4}He. We emphasize that metastable diatomic clusters or DQs can arise only in strong interacting Bose systems at high density and low temperatures. The DQs coupling in liquid ^{4}He for the temperatures below the lambda transition can be explained by the Lennard-Jones intermolecular potential. The ground-state energy E_0 of diatomic clusters or DQ for mass density $\rho = 0.145\ \mathrm{g\,cm^{-3}}$ is given by Eq. (19). This equation yields negative ground-state energy $E_0/k_B = -8.65$ K, which explains the existence of metastable clusters or DQ in liquid ^{4}He for low pressure and temperatures below the lambda transition temperature T_λ. Moreover, it is shown in Secs. IV and V that in liquid ^{4}He for temperature region $1\ \mathrm{K} \leqslant T \leqslant T_\lambda$, diatomic quasiparticles macroscopically populate the ground state which leads to BEC in liquid ^{4}He.

There is no spin interaction in this case because ^{4}He atoms are bosons with zero spin. We note that the pairs of coupled quasiparticles are observed in superfluid ^{3}He with spin $S = 1$ and orbital momentum $L = 1$. In this case, the spin interaction yields the coupling in superfluid ^{3}He, which is also known as spin triplet or odd parity pairing [42–45]. The approach, based on the diatomic quasiparticles concept, yields the critical BEC temperature in liquid ^{4}He as $T_\lambda = 2.16$ K, which is very close to the experimental lambda transition temperature $T_\lambda = 2.17$ K. This theory also leads to superfluid and BEC fractions for liquid ^{4}He which are in good agreement with recent condensation measurements [29–32,46] and Monte Carlo simulations for a wide range of temperatures. Moreover, it is shown in this paper that the condensate fraction for low temperature ($T \leqslant 0.5$ K) at saturated vapor pressure (SVP) is $\rho_0/\rho = 7.22\%$, which is very close to the value $7.25 \pm 0.75\%$ obtained in recent measurements.

In Sec. II, we develop the theory for coupled quasiparticles in liquid ^{4}He for the temperatures below the lambda transition. This many-body approach yields the discrete energy spectrum and effective mass M_q for DQs, which are metastable states of two helium atoms interacting with the atoms of the bulk. We also present in this section the ground-state energy of the DQs. This energy is connected to the roton gap Δ as $E_0 = -\Delta$. In Sec. III, we derive the thermodynamical functions and equation for the critical temperature of BEC in liquid ^{4}He. This equation yields $T_c = 2.16$ K, which is very close to the experimental value of the lambda transition temperature. In Sec. IV, we present the theory of BEC in liquid ^{4}He based on the DQ concept. It is shown that the DQs condense with negative ground-state energy E_0. We also calculate in this section the excited and condensed densities of diatomic quasiparticles and the energy and entropy of DQs for temperature region $T_p \leqslant T \leqslant T_\lambda$ with $T_p \simeq 1$ K. In Secs. V and VI, the superfluid and BEC fractions are calculated for the temperature regions $T_p \leqslant T \leqslant T_\lambda$ and $T \leqslant 0.5$ K, respectively. We show in these sections that theoretical superfluid and BEC fractions are in good agreement with experimental data and Monte Carlo simulations [33–37,47].

II. DIATOMIC QUASIPARTICLES

We describe in this section the spectrum of diatomic quasiparticles in liquid ^{4}He for the temperatures $T_p \leqslant T \leqslant T_\lambda$ with $T_p \simeq 1$ K. The diatomic quasiparticles are defined as the bound states of two helium atoms interacting with particles of the bulk. The DQ concept assumes that the number of diatomic quasiparticles is much less than the number of real particles.

The Hamiltonian for a many-body Bose system with two-particle potential $U(|\mathbf{r}_i - \mathbf{r}_j|)$ is of the form

$$H_N = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}^{N} U(|\mathbf{r}_{ij}|), \tag{1}$$

where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. We assume the commutator relation $[r_{s\alpha}, p_{n\beta}] = i\hbar\delta_{sn}\delta_{\alpha\beta}$, and all other commutators are zero. Here, s, n and α, β are the the particle numbers and projector indexes, respectively. The Hamiltonian in Eq. (1) can also be written as

$$H_N = H_q + H_{N-2}, \tag{2}$$

where H_q is the Hamiltonian for two bound particles with the numbers 1 and 2 interacting with all particles of the bulk, and H_{N-2} is the Hamiltonian for the rest of the particles of a many-body Bose system. It follows from Eq. (1) that the Hamiltonians H_q and H_{N-2} are

$$H_q = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + U(|\mathbf{r}_{12}|) + \sum_{j=3}^{N} U(|\mathbf{r}_{1j}|) + \sum_{j=3}^{N} U(|\mathbf{r}_{2j}|), \tag{3}$$

$$H_{N-2} = \sum_{i=3}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{3\leqslant i<j}^{N} U(|\mathbf{r}_{ij}|). \tag{4}$$

We define the canonical transformation for the operators $\mathbf{r}_s$ and $\mathbf{p}_s$ ($s = 1, 2$) as

$$\mathbf{R} = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \tag{5}$$

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \quad \mathbf{p} = \tfrac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2). \tag{6}$$

The commutation relations for these operators are $[r_\alpha, p_\beta] = i\hbar\delta_{\alpha\beta}$ and $[R_\alpha, P_\beta] = i\hbar\delta_{\alpha\beta}$, and all other commutators are zero. The Hamiltonian given by Eq. (3) can be written as

$$H_q = \frac{1}{2m_c}\mathbf{p}^2 + \frac{1}{2M}\mathbf{P}^2 + \mathcal{U}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2}), \tag{7}$$

where $m_c = m/2$ and $M = 2m$. The potential $\mathcal{U}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2})$ in this equation is of the form

$$\mathcal{U}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2}) = U(|\mathbf{r}|) + \sum_{j=3}^{N} U\left(\left|\mathbf{R} + \tfrac{1}{2}\mathbf{r} - \mathbf{r}_j\right|\right) + \sum_{j=3}^{N} U\left(\left|\mathbf{R} - \tfrac{1}{2}\mathbf{r} - \mathbf{r}_j\right|\right), \tag{8}$$

with $\mathbf{X}_{N-2} = (\mathbf{r}_3, \mathbf{r}_4, \dots, \mathbf{r}_N)$.

The intermolecular interaction for the Bose fluid is given by the Lennard-Jones potential,

$$U(r) = 4\epsilon\left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6}\right], \tag{9}$$

where the minimum of the potential occurs at $r_m = 2^{1/6} r_0$. In the case of a gas or liquid ^{4}He to good accuracy, the parameters of the Lennard-Jones potential are calculated by the self-consistent-field Hartree-Fock method. It is shown that the parameters are given by $\epsilon/k_B = 10.6$ K and $r_m = 2.98 \times 10^{-8}$ cm [48]. The quantum-chemical methods produce very accurate potential energy curves for van der Waals molecules, which is demonstrated through the calculation of helium dimer interaction energy for a variety of internuclear distances [49]. These results are in close agreement with Ref. [48] and the empirical potential of Aziz *et al.* [50].

In this section, we use the Schrödinger representation for operators. The potential in Eq. (8) can be written as

$$\mathcal{U}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2}) = \bar{\mathcal{U}}(\mathbf{R}, \mathbf{r}) + \mathcal{V}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2}), \tag{10}$$

where $\bar{\mathcal{U}}(\mathbf{R}, \mathbf{r}) = \langle \mathcal{U}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2}) \rangle_{N-2}$ is the potential averaged by the density matrix over the position of $N-2$ particles with the numbers $3, 4, \dots, N$. The function $\mathcal{V}(\mathbf{R}\,\mathbf{r}, \mathbf{X}_{N-2})$ describes the fluctuations of the potential in Eq. (10) with $\langle \mathcal{V}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2}) \rangle_{N-2} = 0$. The decomposition of average potential $\bar{\mathcal{U}}(\mathbf{R}, \mathbf{r})$ of the quasiparticle in a series around an equilibrium position with $\mathbf{R} = \mathbf{R}_0$ and $r = r_0$ has the form

$$\bar{\mathcal{U}}(\mathbf{R}, \mathbf{r}) = \bar{\mathcal{U}}_0 + \frac{1}{2} m_c \omega_0^2 (r - r_0)^2 + \sum_{s=1}^{3} \frac{1}{2} M_q \omega_s^2 (R_s - R_{0s})^2 + \cdots, \tag{11}$$

where $\bar{\mathcal{U}}_0 = \bar{\mathcal{U}}(\mathbf{R}_0, \mathbf{n} r_0)$ and $\mathbf{n} = \mathbf{r}/r$ is the unit vector. The frequencies are given by $\omega_0^2 = m_c^{-1} \partial_r^2 \bar{\mathcal{U}}(\mathbf{R}_0, \mathbf{n} r)|_{r=r_0}$ and $\omega_s^2 = M_q^{-1} \partial_{R_s}^2 \bar{\mathcal{U}}(\mathbf{R}, \mathbf{n} r_0)|_{\mathbf{R}=\mathbf{R}_0}$ for $s = 1, 2, 3$, respectively. We use, in this decomposition, the renormalized mass $M_q = \sigma M$ for diatomic quasiparticles. The factor is $\sigma = 2^{2/3}$ (see Appendix A) and hence the renormalized mass is given by $M_q = \sigma M = 2^{5/3} m$. We also note that the frequency ω_s depends on the temperature and density of the Bose liquid.

The DQ Hamiltonian can be written by Eqs. (7), (10), and (11) in the form

$$H_q = \bar{\mathcal{U}}_0 + H_q^{(1)} + H_q^{(2)} + \mathcal{V}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2}), \tag{12}$$

where the Hamiltonians $H_q^{(1)}$ and $H_q^{(2)}$ are

$$H_q^{(1)} = -\frac{\hbar^2}{2m_c} \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{2} m_c \omega_0^2 (r - r_0)^2 + \frac{\hbar^2}{2m_c r_0^2} J(J+1), \tag{13}$$

$$H_q^{(2)} = -\frac{\hbar^2}{2M_q} \sum_{s=1}^{3} \frac{\partial^2}{\partial R_s^2} + \sum_{s=1}^{3} \frac{1}{2} M_q \omega_s^2 \left(R_s - R_{0s}\right)^2. \tag{14}$$

The Hamiltonian in Eq. (13) describing the internal degrees of freedom of the DQ is written in a spherical coordinate system. We note that the term $\mathcal{V}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2})$ is connected with the fluctuation of interactions in Eq. (12), and it can be neglected for the eigenenergy problem to a good accuracy. The effective Hamiltonian $H_q^{(1)}$ describes the internal 1D vibrations and rotations of DQ and the Hamiltonian $H_q^{(2)}$ describes three-dimensional (3D) harmonic vibrations for the center of mass of DQ with effective mass M_q. The discrete energy spectrums follow from the Hamiltonians $H_q^{(1)}$ and $H_q^{(2)}$ as $E_{n_0 \mathrm{J}}^{(1)} = (\hbar^2/2m_c r_0^2) J(J+1) + \hbar\omega_0 (n_0 + 1/2)$ and $E_{n_1 n_2 n_3}^{(2)} = \sum_{s=1}^{3} \hbar\omega_s (n_s + 1/2)$, respectively, where $J = 0, 1, 2, \dots$ and $n_s = 0, 1, 2, \dots$ with $s = 0, 1, 2, 3$. However, the rotations of the DQ are "frozen" in the liquid at low temperatures. Hence, the angular momentum quantum number is $J = 0$. Moreover, one can choose the third Cartesian axis as $\mathbf{e}_3 = \mathbf{n}$; then the average potential $\bar{\mathcal{U}}(\mathbf{R}, \mathbf{n} r)$ yields the relation $\omega_1 = \omega_2$ for the frequencies. The discrete eigenenergies for the Hamiltonian H_q are

$$E_{n_0 n_1 n_2 n_3} = \bar{\mathcal{U}}_0 + E_{n_0 0}^{(1)} + E_{n_1 n_2 n_3}^{(2)} = E_0 + \sum_{s=0}^{3} \hbar\omega_s n_s, \tag{15}$$

where $E_0 = \bar{\mathcal{U}}_0 + \sum_{s=0}^{3} \frac{1}{2} \hbar\omega_s$ is the energy of the ground state of the DQ. We note that the DQ states with the energies $E_{n_0 n_1 n_2 n_3}$ are metastable because the fluctuation of the interaction given by the term $\mathcal{V}(\mathbf{R}, \mathbf{r}, \mathbf{X}_{N-2})$ leads to collisions of a pair of bound atoms with the surrounding atoms. There is also another scattering channel which corresponds to the dissociation of DQs. The energy spectrum of Hamiltonian H_q also has the continuous component given by

$$\varepsilon_q(\mathbf{p}) = \epsilon_q + \frac{\mathbf{p}^2}{2M_q}, \tag{16}$$

where $\mathbf{p}$ is the momentum of the DQ. Equation (8) yields the average potential energy in the form $\bar{\mathcal{U}}(\mathbf{R}, \mathbf{r}) = U(r) + W(\mathbf{R}, \mathbf{r})$, where the function $W(\mathbf{R}, \mathbf{r})$ is given by

$$W(\mathbf{R}, \mathbf{r}) = \left\langle \left[U\left(\left|\mathbf{R} + \tfrac{1}{2}\mathbf{r} - \mathbf{r}'\right|\right) + U\left(\left|\mathbf{R} - \tfrac{1}{2}\mathbf{r} - \mathbf{r}'\right|\right)\right]\right\rangle_{\mathbf{r}'}. \tag{17}$$

Here, $\langle \cdot \rangle_{\mathbf{r}'}$ is the averaging to variable $\mathbf{r}'$ with a conditional distribution. The position of the atoms in the DQ is given by $\mathbf{r}_1 = \mathbf{R} + \frac{1}{2}\mathbf{r}$ and $\mathbf{r}_2 = \mathbf{R} - \frac{1}{2}\mathbf{r}$. It follows from Eq. (17) that function $W(\mathbf{R}, \mathbf{r})$ is invariant to the change $\mathbf{r}_1 \to \mathbf{r}_2$ and $\mathbf{r}_2 \to \mathbf{r}_1$.

The inequality $\hbar\omega_s \ll |E_0|$ (see Appendix B) yields the relation $W(\mathbf{R}, \mathbf{n} r_m) \simeq W(\mathbf{R}, \mathbf{n} r_a)$, where $r_m = 2^{1/6} r_0$, and $r_a = 2a_0$ at low pressures [19]. Here, a_0 is the s-scattering length of helium atoms. Thus, the ground-state energy of the DQ is

$$E_0 = \bar{\mathcal{U}}(\mathbf{R}, \mathbf{n}r_m) - \bar{\mathcal{U}}(\mathbf{R}, \mathbf{n}r_a) \simeq U(r_m) - U(r_a)$$
$$= -4\epsilon\left[\frac{1}{4} - \left(\frac{r_0}{r_a}\right)^6 + \left(\frac{r_0}{r_a}\right)^{12}\right]. \tag{18}$$

The relation $r_a = 2a_0$ is connected to the s-scattering cross section $\sigma_s = 4\pi a_0^2$ for helium atoms. We note that the s-scattering length for ^{4}He atoms is $a_0 = 2.2 \times 10^{-8}$ cm [19]. Moreover, the distance r_a is close to the average distance $\bar{r} = 2(3m/4\pi\rho)^{1/3}$ between the atoms in a Bose liquid at low pressure. Hence, for enough low pressures, we have the relation $r_a = a\bar{r}$. This equation leads to ground-state energy E_0 of the DQs, which is a function of mass density ρ. The constant parameter a can be defined as $a = 2a_0/\bar{r}$, where the average distance $\bar{r}$ is given for the mass density $\rho = 0.145$ g cm^{-3}. In this case, the average distance is $\bar{r} = 4.44 \times 10^{-8}$ cm and the constant parameter $a = 2a_0/\bar{r}$ is given as $a = 0.991$.

Equation (18) leads to the ground-state energy of the DQs, which is a function of mass density,

$$E_0(\rho) = -\epsilon\left[1 - 4\left(\frac{\rho}{\rho_a}\right)^2 + 4\left(\frac{\rho}{\rho_a}\right)^4\right], \quad \rho_a = \frac{6ma^3}{\pi r_0^3}. \tag{19}$$

We note that for low pressure, the mass density is $\rho = 0.145$ g cm^{-3}, and hence Eq. (19) yields $E_0/k_B = -8.65$ K for the parameters presented in Ref. [48]. The empirical potential given in Ref. [50] leads to a very close normalized ground-state energy of the DQs as $E_0/k_B = -8.594$ K. Moreover, it is shown in Ref. [19] that the roton gap Δ in liquid ^{4}He is connected to the ground-state energy of the DQs by relation $\Delta = -E_0$.

III. LAMBDA TRANSITION TEMPERATURE IN LIQUID ^{4}He

In this section, we derive the equations for the average energy, free energy, and entropy for the trapped DQ in liquid ^{4}He. We also derive the equation for the lambda transition temperature which agrees, to a high accuracy, with experimental temperature T_λ for liquid ^{4}He. This temperature is found to be a necessary condition for the lambda transition in liquid ^{4}He. It is shown in the following section that this condition is sufficient as well. We also show in Sec. V that the mass density of the DQs is much smaller than the mass density ρ in liquid ^{4}He. In this case, the probability that a trapped DQ has the vibrational energy $E_{n_0n_1n_2n_3}$ is given by

$$\mathcal{P}_{n_0n_1n_2n_3}(\beta) = \frac{1}{\mathcal{Z}(\beta)}\exp(-\beta E_{n_0n_1n_2n_3}), \tag{20}$$

where $\beta = 1/k_BT$ and the partition function $\mathcal{Z}(\beta)$ is

$$\mathcal{Z}(\beta) = \sum_{n_0=0}^{\infty}\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty}\exp(-\beta E_{n_0n_1n_2n_3}). \tag{21}$$

We note that the discrete energy spectrum in Eq. (15) is accurate only for enough small quantum numbers n_s. However, the partition function in Eq. (21) is given to good accuracy because the terms with large numbers n_s are small when $T \leqslant T_\lambda$. The calculation of the sums in Eq. (21) leads to the equation for partition function $\mathcal{Z}(\beta)$ as

$$\ln\mathcal{Z}(\beta) = -\beta E_0 - \sum_{s=0}^{3}\ln[1 - \exp(-\beta\varepsilon_s)], \tag{22}$$

with $\varepsilon_s = \hbar\omega_s$. Thus, the average energy of the DQ and dispersion of energy are

$$\bar{E}_q(\beta) = -\frac{\partial}{\partial\beta}\ln\mathcal{Z}(\beta) = E_0 + \sum_{s=0}^{3}\frac{\varepsilon_s}{\exp(\beta\varepsilon_s) - 1}, \tag{23}$$

$$D_q(\beta) = \frac{\partial^2}{\partial\beta^2}\ln\mathcal{Z}(\beta) = \sum_{s=0}^{3}\frac{\varepsilon_s^2\exp(\beta\varepsilon_s)}{[\exp(\beta\varepsilon_s) - 1]^2}. \tag{24}$$

The free energy and entropy of the DQ are given by

$$F_q(\beta) = -\frac{1}{\beta}\ln\mathcal{Z}(\beta) = E_0 + \frac{1}{\beta}\sum_{s=0}^{3}\ln[1 - \exp(-\beta\varepsilon_s)], \tag{25}$$

$$S_q(\beta) = -\frac{\partial}{\partial T}F_q(\beta) = T^{-1}[\bar{E}_q(\beta) - F_q(\beta)]. \tag{26}$$

These equations can be simplified for the temperatures $T \simeq T_\lambda$. We show in Appendix B that the following inequality is satisfied for liquid ^{4}He:

$$\beta_\lambda\varepsilon_s = \frac{\hbar\omega_s}{k_BT_\lambda} \ll 1, \quad s = 0, 1, 2, 3. \tag{27}$$

Thus, for temperatures $T \simeq T_\lambda$, Eqs. (23) and (24) can be written as

$$\bar{E}_q(\beta) = E_0 + 4k_BT, \tag{28}$$

$$\Delta_q(\beta) = \sqrt{D_q(\beta)} = 2k_BT, \tag{29}$$

where $\Delta_q(\beta)$ is the energy variation. In the case $T \simeq T_\lambda$, free energy and entropy of the DQ are given by

$$F_q(\beta) = E_0 + k_BT\sum_{s=0}^{3}\ln\frac{\varepsilon_s}{k_BT}, \tag{30}$$

$$S_q(\beta) = 4k_B - k_B\sum_{s=0}^{3}\ln\frac{\varepsilon_s}{k_BT}. \tag{31}$$

These equations lead to the entropy differential as

$$dS_q(\beta) = \frac{4k_BdT}{T} = \frac{d\bar{E}_q(\beta)}{T}. \tag{32}$$

The necessary condition for the existence of a finite fraction of trapped DQs in liquid ^{4}He is $\bar{E}_q(\beta) < 0$, which can be written by Eq. (28) as $E_0 + 4k_BT < 0$. Thus, the trapped DQs have finite fraction in liquid ^{4}He when the condition $T < |E_0|/4k_B$ is satisfied. We show in the following section that this condition is also a sufficient condition for the lambda transition in liquid ^{4}He. Hence, the critical temperature for BEC in liquid ^{4}He is given by

$$T_c = \frac{|E_0(\rho)|}{4k_B}, \tag{33}$$

where the energy $|E_0|$ is defined by Eq. (19) as

$$|E_0(\rho)| = \epsilon\left[1 - 4\left(\frac{\rho}{\rho_a}\right)^2 + 4\left(\frac{\rho}{\rho_a}\right)^4\right]. \quad (34)$$

It is accepted that the critical temperature for BEC in liquid ^{4}He is equal to the lambda transition temperature [12]. Equation (34) yields $|E_0|/k_B = 8.65$ K for low pressure or the helium mass density $\rho = 0.145$ g cm^{-3}. Hence, in this case, Eq. (33) leads to the critical BEC temperature as $T_c = T_\lambda = 2.16$ K, which is in excellent agreement with the experimental lambda transition temperature given by $T_\lambda = 2.17$ K. The lambda transition temperature and critical BEC temperature in Eqs. (33) and (34) are the functions of mass density as

$$T_\lambda(\rho) = T_c(\rho) = \frac{\epsilon}{k_B}\left[\frac{1}{4} - \left(\frac{\rho}{\rho_a}\right)^2 + \left(\frac{\rho}{\rho_a}\right)^4\right], \quad (35)$$

where $\rho_a = 6ma^3/\pi r_0^3$. The developed theory does not apply to dilute Bose gas because the DQs exist only in liquid ^{4}He at low temperatures. We emphasize that the parameters $\epsilon/k_B = 10.63$ K and $r_m = 2.96 \times 10^{-8}$ cm presented in the paper [49] lead to normalized ground-state energy of DQs and the lambda transition temperature as $E_0/k_B = -8.7$ K and $T_\lambda = 2.175$ K. Thus, the normalized ground-state energy of DQs and the lambda transition temperature obtained by parameters presented in Refs. [48,50] (see the end of Sec. II) are in good agreement with the above result. This shows that two interacting atoms in a liquid ^{4}He have negative energy and hence they can form a bound state at low pressure and enough low temperature.

IV. BEC CONDENSATION IN BOSE FLUIDS

In this section, we develop the theory of BEC in liquid ^{4}He for temperature region $T_p \leqslant T \leqslant T_\lambda$ where the bound temperature is $T_p \simeq 1$ K. The DQs in this temperature region can be described as a Bose system consisting of two fractions. The first fraction is a Bose gas of DQs with the continuous energy spectrum given by Eq. (16) and the second fraction consists of trapped DQs with a discrete energy spectrum given in Eq. (15).

The full Hamiltonian for the liquid Bose fluid can be written in the form

$$\hat{H} = \hat{H}_q + \hat{H}_a + \hat{H}_{\text{int}}, \quad (36)$$

where $\hat{H}_q$ is the Hamiltonian describing DQs in liquid ^{4}He, and $\hat{H}_a$ is the Hamiltonian for the rest of the free quasiparticles, including the rotons and phonons. The Hamiltonian $\hat{H}_{\text{int}}$ describes the interaction of all sorts of quasiparticles in the Bose fluid.

The concept of the quasiparticles assumes that the number of quasiparticle excitations is much less than the number of real particles. Thus the DQ's subsystem can be described as two fractions: an ideal Bose gas of DQs with the continuous energy spectrum and the fraction of DQs with a discrete energy spectrum. We emphasize that in this representation of quasiparticles, the interaction energy of the DQs is much less than their full energy. Thus, the DQs are weakly interacting excitations in a liquid Bose fluid. We show in Sec. V that this picture leads to good agreement with the experimental data.

Using the results of Sec. II, we can write the Hamiltonian for two components of DQs as

$$\hat{H}_q = \sum_{\mathbf{p}} \varepsilon_q(\mathbf{p})\hat{d}^\dagger(\mathbf{p})\hat{d}(\mathbf{p}) + \sum_{n_0}\sum_{n_1}\sum_{n_2}\sum_{n_3} \delta_{\{n\}}E_{\{n\}}\hat{d}^\dagger_{\{n\}}\hat{d}_{\{n\}}, \quad (37)$$

where $E_{\{n\}} = E_{n_0n_1n_2n_3}$ is the discrete energy spectrum given by Eq. (15) and $\varepsilon_q(\mathbf{p}) = \epsilon_q + \mathbf{p}^2/2M_q$ is the continuous energy spectrum of DQs with $|\epsilon_q| \ll |E_0|$. The operators $\hat{d}^\dagger_{\{n\}}$, $\hat{d}_{\{n\}}$, $\hat{d}^\dagger(\mathbf{p})$, $\hat{d}(\mathbf{p})$ are creation and annihilation Bose operators for discrete and continuous energy spectrums of DQs, respectively. The function $\delta_{\{n\}}$ is defined as $\delta_{\{n\}} = 1$ when $E_{\{n\}} < 0$, and $\delta_{\{n\}} = 0$ otherwise. The number operators of DQs for discrete and continuous energy spectrums have the form

$$\hat{N}_0 = \sum_{n_0}\sum_{n_1}\sum_{n_2}\sum_{n_3} \delta_{\{n\}}\hat{d}^\dagger_{\{n\}}\hat{d}_{\{n\}}, \quad (38)$$

$$\hat{N}_1 = \sum_{\mathbf{p}} \hat{d}^\dagger(\mathbf{p})\hat{d}(\mathbf{p}) = \sum_{\mathbf{p}} \hat{N}_1(\mathbf{p}), \quad (39)$$

where $\hat{N}_1(\mathbf{p}) = \hat{d}^\dagger(\mathbf{p})\hat{d}(\mathbf{p})$ and $\hat{N}_q = \hat{N}_0 + \hat{N}_1$ is the full number operator for the DQs.

The grand canonical density operator for the DQs' subsystem is

$$\hat{\rho}_q = \Xi_q^{-1}\exp[-\beta(\hat{H}_q - \mu_0\hat{N}_0 - \mu_1\hat{N}_1)], \quad (40)$$

where the grand canonical partition function is

$$\Xi_q = \mathrm{Tr}\exp[-\beta(\hat{H}_q - \mu_0\hat{N}_0 - \mu_1\hat{N}_1)]. \quad (41)$$

The chemical potentials μ_0 and μ_1 are equal, $\mu_0 = \mu_1 = \tilde{\mu}$. Hence, the average number $\tilde{N}_1(\mathbf{p}) = \langle\hat{N}_1(\mathbf{p})\rangle$ of DQs with the momenta $\mathbf{p}$ is given by

$$\tilde{N}_1(\mathbf{p}) = \frac{1}{\exp\{\beta[\varepsilon_q(\mathbf{p}) - \tilde{\mu}]\} - 1}. \quad (42)$$

The average number $\tilde{N}_0 = \langle\hat{N}_0\rangle$ of DQs for the discrete energy spectrum is

$$\tilde{N}_0 = \sum_{n_0}\sum_{n_1}\sum_{n_2}\sum_{n_3} \frac{\delta_{\{n\}}}{\exp[\beta(E_{\{n\}} - \tilde{\mu})] - 1}. \quad (43)$$

Thus, the full average number $\tilde{N}_q$ of DQs is given by

$$\tilde{N}_q = \tilde{N}_0 + \tilde{N}_1, \quad \tilde{N}_1 = \sum_{\mathbf{p}} \tilde{N}_1(\mathbf{p}). \quad (44)$$

The average number $\tilde{N}_c$ of DQs in the ground state with energy E_0 is

$$\tilde{N}_c = \frac{1}{\exp[\beta(E_0 - \tilde{\mu})] - 1}. \quad (45)$$

The density of the DQs in the ground state is $\tilde{n}_c = \mathrm{Lim}(\tilde{N}_c/V)$, where Lim denotes the thermodynamical limit ($N, V \to \infty$ for $N/V = n =$ const). Here, N is the full number of atoms in volume V. It follow from Eqs. (42) and (43) (see, also, Appendix C) that the full density of the DQs is

$$\frac{\tilde{N}_q}{V}=\left(\frac{M_q}{2\pi\hbar^2\beta}\right)^{3/2}\zeta_{3/2}[\exp(\beta\tilde{\mu})]+\frac{1}{V}\sum_{\{n\}}\frac{\delta_{\{n\}}}{\exp[\beta(E_{\{n\}}-\tilde{\mu})]-1},\tag{46}$$

where the first and second terms are $\tilde{N}_1/V$ and $\tilde{N}_0/V$, respectively. The function $\zeta_s(z)$ is a polylogarithm; this is a generalization of the Riemann zeta function given by

$$\zeta_s(z)\equiv \mathrm{Li}_s(z)=\sum_{n=1}^{\infty}\frac{z^n}{n^s}.$$

The chemical potential $\tilde{\mu}$ is a volume-dependent function. We also define the chemical potential $\mu=\mathrm{Lim}\ \tilde{\mu}$, which is a limiting case of chemical potential $\tilde{\mu}$. It follows from Eq. (46) that $\mu=E_0$ for low temperatures when $T<T_c$. The critical temperature T_c for fixed density $\tilde{n}_q$ follows from

$$\tilde{n}_q=\left(\frac{M_qk_BT_c}{2\pi\hbar^2}\right)^{3/2}\zeta_{3/2}(z_c),\quad z_c=\exp\left(\frac{E_0}{k_BT_c}\right).\tag{47}$$

Equation (46) also yields $\tilde{n}_q=\tilde{n}_0+\tilde{n}_1$, where $\tilde{n}_0=\mathrm{Lim}(\tilde{N}_0/V)$ and $\tilde{n}_1=\mathrm{Lim}(\tilde{N}_1/V)$, and the density $\tilde{n}_1$ for $T<T_c$ is given by

$$\tilde{n}_1=\left(\frac{M_q}{2\pi\hbar^2\beta}\right)^{3/2}\zeta_{3/2}[\exp(\beta E_0)].\tag{48}$$

Below, we present the theorem which defines the volume-dependent chemical potential $\tilde{\mu}$ in the range of temperatures $T\leqslant T_c$. It is important that this equation for the volume-dependent chemical potential $\tilde{\mu}$ leads to the correct thermodynamical limit for the condensed fraction.

Theorem: The chemical potential $\tilde{\mu}$ for the arbitrary fixed density $\tilde{n}_q$ in the range of temperatures $T<T_c$ is

$$\tilde{\mu}(\tilde{n}_q,T,V)=\mu-k_BT\left(\tilde{N}_c^{-1}-\frac{1}{2}\tilde{N}_c^{-2}+\frac{1}{3}\tilde{N}_c^{-3}-\cdots\right),\tag{49}$$

where $\mu=E_0$, $\tilde{N}_c=(\tilde{n}_q-\tilde{n}_1)V$, and the volume V is sufficient large that $(\tilde{n}_q-\tilde{n}_1)V\gg 1$. The densities $\tilde{n}_q$ and $\tilde{n}_1$ are given by Eqs. (47) and (48), where $\tilde{n}_q=\tilde{n}_0+\tilde{n}_1$, and $\tilde{n}_0=\tilde{n}_c>0$ for $T<T_c$. The chemical potential $\tilde{\mu}$ for the critical temperature T_c has the form $\tilde{\mu}=E_0-\varepsilon$, where $\varepsilon>0$.

It is accepted here that the limit $\varepsilon\to 0$ always follows after the thermodynamical limit. First we show that Eq. (49) yields the correct density $\tilde{n}_0$ in the thermodynamical limit. Equations (43) and (49) lead to the following equations:

$$\begin{aligned}\frac{\tilde{N}_0}{V}&=\sum_{\{n\}}\frac{\delta_{\{n\}}V^{-1}}{\exp[\beta(E_{\{n\}}-\tilde{\mu})]-1}\simeq\frac{V^{-1}}{\exp[\beta(E_0-\tilde{\mu})]-1}\\&\simeq\frac{V^{-1}}{\exp[1/(\tilde{n}_q-\tilde{n}_1)V]-1}\simeq\tilde{n}_q-\tilde{n}_1,\end{aligned}\tag{50}$$

where we can use decomposition $\exp(1/X)=1+X^{-1}+(1/2)X^{-2}+\cdots$ for $X=(\tilde{n}_q-\tilde{n}_1)V\gg 1$. Thus, for the range of temperatures $T<T_c$, Eqs. (48) and (50) yield, for the thermodynamical limit, the following equation:

$$\tilde{n}_q=\tilde{n}_0+\left(\frac{M_q}{2\pi\hbar^2\beta}\right)^{3/2}\zeta_{3/2}[\exp(\beta E_0)].\tag{51}$$

Equation (45) yields the necessary condition for volume-dependent chemical potential $\tilde{\mu}$. It leads to the following decomposition:

$$\begin{aligned}\tilde{\mu}&=E_0-k_BT\ \ln(1+\tilde{N}_c^{-1})\\&=E_0-k_BT\left(\tilde{N}_c^{-1}-\frac{1}{2}\tilde{N}_c^{-2}+\frac{1}{3}\tilde{N}_c^{-3}-\cdots\right),\end{aligned}\tag{52}$$

where $E_0=\mu$ and $\tilde{N}_c\gg 1$. Moreover, Eqs. (43) and (45) yield relation $\tilde{n}_0=\tilde{n}_c$. Thus, Eq. (49) is valid when the condition $\tilde{N}_c=(\tilde{n}_q-\tilde{n}_1)V\gg 1$ is satisfied.

It follows from Eq. (51) that the full density of the DQs is $\tilde{n}_q=\tilde{n}_0+\tilde{n}_1$, where $\tilde{n}_0=\tilde{n}_c>0$ for the range of temperatures $T<T_c$, and $\tilde{n}_0=\tilde{n}_c=0$ when $T\geqslant T_c$. Hence, the DQs condense in the ground state with energy E_0 for the range of temperatures $T<T_c$.

Equation (42) yields the excitation density $\tilde{n}_1$ as

$$\tilde{n}_1=\frac{1}{(2\pi\hbar)^3}\int\frac{1}{\exp\{\beta[\varepsilon_q(\mathbf{p})-E_0]\}-1}d\mathbf{p}.\tag{53}$$

We note that for the temperature region $T_p<T<T_\lambda$ with $T_p\simeq 1$, an inequality $e^{-\beta\mu}=e^{\beta|E_0|}\gg 1$ is satisfied because the ground-state energy of the DQs is $E_0/k_B=-8.65$ K (see Sec. II).

Equation (53) for condition $e^{\beta|E_0|}\gg 1$ has the form $\tilde{n}_1=\int f_q(\mathbf{p})d\mathbf{p}$, where the momentum distribution of the diatomic quasiparticles is

$$f_q(\mathbf{p})=\frac{1}{(2\pi\hbar)^3}\exp\{-\beta[\varepsilon_q(\mathbf{p})-E_0]\}.\tag{54}$$

Integration in Eq. (53) for conditions $|\epsilon_q|\ll|E_0|$ and $e^{\beta|E_0|}\gg 1$ leads to the excitation density of the DQs as

$$\tilde{n}_1(T,\rho)=\frac{1}{\lambda_q^3(T)}\exp\left(-\frac{|E_0(\rho)|}{k_BT}\right),\tag{55}$$

where the thermal wavelength $\lambda_q(T)$ is

$$\lambda_q(T)=\left(\frac{2\pi\hbar^2}{M_qk_BT}\right)^{1/2}.\tag{56}$$

We note that Eq. (55) also follows from Eq. (48) when the condition $e^{\beta|E_0|}\gg 1$ is satisfied. Relation $\tilde{n}_0=\tilde{n}_c$ and Eq. (51) yield the condensate density as

$$\tilde{n}_0(T,\rho)=\tilde{n}_c(T,\rho)=\tilde{n}_q(\rho)-\tilde{n}_1(T,\rho).\tag{57}$$

Hence, equation $\tilde{n}_1=\tilde{n}_q$ is satisfied for critical temperature T_c.

Equation (55) for temperature T_c and Eq. (33) yield the full density of the diatomic quasiparticles as

$$\tilde{n}_q(\rho)=e^{-4}\left(\frac{M_qk_BT_c(\rho)}{2\pi\hbar^2}\right)^{3/2}=e^{-4}\left(\frac{M_q|E_0(\rho)|}{8\pi\hbar^2}\right)^{3/2},\tag{58}$$

where the functions $T_c(\rho)$ and $|E_0(\rho)|$ are presented by Eqs. (35) and (34), respectively. We emphasize that Eq. (58) yields an inequality $\tilde{n}_q/n\ll 1$, where $n=\mathrm{Lim}\ N/V$ is the density of atoms in liquid ^{4}He. Thus, the necessary condition for the theory based on the DQs concept is satisfied.

Equation (58) leads to the critical temperature for a BEC in liquid ^{4}He as

$$T_c(\rho) = \frac{2\pi e^{8/3}\hbar^2 \tilde{n}_q(\rho)^{2/3}}{k_B M_q} = \frac{|E_0(\rho)|}{4k_B}. \tag{59}$$

We note that the energy density $\mathcal{U}_q = \mathrm{Lim}(U_q/V)$ (for details, see Appendix C) of the diatomic quasiparticles can be written by Eq. (C8) in the form

$$\mathcal{U}_q(T,\rho) = \tfrac{3}{2}k_B T \tilde{n}_1(T,\rho) + E_0(\rho)[\tilde{n}_q(\rho) - \tilde{n}_1(T,\rho)]. \tag{60}$$

The entropy density of the diatomic quasiparticles follows from Eq. (C9) as

$$\mathcal{S}_q(T,\rho) = \mathrm{Lim}\frac{S_q}{V} = \left(\frac{5}{2}k_B + \frac{|E_0(\rho)|}{T}\right)\tilde{n}_1(T,\rho). \tag{61}$$

Equations (60) and (61) lead to free energy density $\mathcal{F}_q = \mathcal{U}_q - T\mathcal{S}_q$ of the diatomic quasiparticles,

$$\mathcal{F}_q(T,\rho) = E_0(\rho)\tilde{n}_q(\rho) - k_B T \tilde{n}_1(T,\rho). \tag{62}$$

We emphasize that equations $\Delta = -E_0$ and $\mu_{\mathrm{rot}} = -\Delta$, where Δ and μ_{rot} are the roton gap and roton chemical potential, are found in Ref. [19]. Furthermore, the theorem proven in this section yields $\mathrm{Lim}\,\tilde{\mu} = \mu = E_0$, where the ground-state energy of the DQs is given by Eq. (19). These equations lead to general relation $\mu = \mu_{\mathrm{rot}} = E_0$ for the temperature region $T_p \leqslant T \leqslant T_\lambda$.

V. SUPERFLUID AND BEC FRACTIONS IN LIQUID ^{4}He FOR TEMPERATURES $T_p \leqslant T \leqslant T_\lambda$

In this section, we derive the fractions of BEC and superfluid fractions in liquid ^{4}He for temperatures $T_p \leqslant T \leqslant T_\lambda$ with $T_p \simeq 1$ K. We also show that these superfluid and BEC fractions are in good agreement with experimental data and Monte Carlo simulations [36,47]. We note that in the temperature interval $T_p \leqslant T \leqslant T_\lambda$, there exist three types of quasiparticles: diatomic quasiparticles, rotons, and phonons. Moreover, we show that the superfluid and BEC fractions in liquid ^{4}He are completely defined by thermodynamical functions for the diatomic quasiparticles in the temperature region $T_p \leqslant T \leqslant T_\lambda$.

The full mass density of the DQs and mass densities for condensed and excited quasiparticles are given as $\rho_q = M_q\tilde{n}_q$, $\rho_0 = M_q\tilde{n}_0$, and $\rho_1 = M_q\tilde{n}_1$, respectively. The condensate fraction in a liquid Bose fluid for the temperature region $T_p \leqslant T \leqslant T_\lambda$ is given as $\rho_0/\rho = (\tilde{n}_q - \tilde{n}_1)M_q/\rho$. Equations (55), (58), and (59) and relation $T_c = T_\lambda$ yield

$$\frac{\rho_0}{\rho} = f(\rho)[1 - \Phi(T,\rho)], \tag{63}$$

$$\frac{\rho_1}{\rho} = f(\rho)\Phi(T,\rho). \tag{64}$$

The functions $f(\rho)$ and $\Phi(T,\rho)$ are given by

$$f(\rho) = \frac{M_q}{e^4\rho}\left(\frac{M_q k_B T_\lambda(\rho)}{2\pi\hbar^2}\right)^{3/2}, \tag{65}$$

$$\Phi(T,\rho) = \left(\frac{T}{T_\lambda(\rho)}\right)^{3/2}\exp\left[4\left(1 - \frac{T_\lambda(\rho)}{T}\right)\right], \tag{66}$$

where lambda transition temperature $T_\lambda(\rho)$ is a function of the density given in Eq. (35). We emphasize that the excitation mass density $\rho_1 = \rho_q - \rho_0$ is connected to the full density ρ_q of the diatomic quasiparticles. We can also introduce the full excitation mass density by relation $\rho_{\mathrm{ex}} = \rho - \rho_0$; then the full excitation fraction is

$$\frac{\rho_{\mathrm{ex}}}{\rho} = 1 - f(\rho)[1 - \Phi(T,\rho)]. \tag{67}$$

Equations (63) and (67) lead to the relation $\rho_{\mathrm{ex}}/\rho + \rho_0/\rho = 1$.

The energy density of the diatomic quasiparticles can be written in normalized form $\tilde{\mathcal{U}}_q = \mathcal{U}_q(T)/\mathcal{U}_q(T_\lambda)$, where the energy density $\mathcal{U}_q(T)$ is given by Eq. (60) and $\mathcal{U}_q(T_\lambda) = (3/2)k_B T_\lambda \tilde{n}_q$. This definition leads to the normalized energy density as

$$\tilde{\mathcal{U}}_q(T,\rho) = \left(\frac{8}{3} + \frac{T}{T_\lambda(\rho)}\right)\Phi(T,\rho) - \frac{8}{3}. \tag{68}$$

The normalized entropy density of the diatomic quasiparticles is $\tilde{\mathcal{S}}_q = \mathcal{S}_q(T)/\mathcal{S}_q(T_\lambda)$, where the entropy density $\mathcal{S}_q(T)$ is given by Eq. (61) and $\mathcal{S}_q(T_\lambda) = (13/2)k_B\tilde{n}_q$. Hence, the normalized entropy density of the diatomic quasiparticles is

$$\tilde{\mathcal{S}}_q(T,\rho) = \left[\frac{5}{13} + \frac{8}{13}\left(\frac{T_\lambda(\rho)}{T}\right)\right]\Phi(T,\rho). \tag{69}$$

We have two different equations for densities in the temperature interval $T_p \leqslant T \leqslant T_\lambda$ as

$$\rho_q = \rho_0 + \rho_1, \quad \rho = \rho_s + \rho_n, \tag{70}$$

where the second equation is written for the superfluid ρ_s and normal ρ_n mass densities. We can also write, for this temperature region, the following equation: $\rho_1 = \alpha(\rho)\rho_n$, where $\alpha(\rho)$ is some function of density ρ. Hence, relations $\rho_1 = \rho_q$ and $\rho_n = \rho$ for temperature $T = T_\lambda$ yield equation $\rho_q = \alpha(\rho)\rho$. Moreover, Eq. (70) and relations $\rho_1 = \alpha(\rho)\rho_n$ and $\rho_q = \alpha(\rho)\rho$ lead to equation $\rho_0 = \alpha(\rho)\rho_s$. Thus, for the temperature region $T_p \leqslant T \leqslant T_\lambda$, we have the following equations:

$$\frac{\rho_1}{\rho} = \alpha(\rho)\frac{\rho_n}{\rho}, \quad \frac{\rho_0}{\rho} = \alpha(\rho)\frac{\rho_s}{\rho}, \tag{71}$$

where $\alpha(\rho) = \rho_q(\rho)/\rho$. Equation (71) and relation $\rho_{\mathrm{ex}}/\rho = 1 - \rho_0/\rho$ lead to another important equation,

$$\frac{\rho_{\mathrm{ex}}}{\rho} = 1 - \alpha(\rho) + \alpha(\rho)\frac{\rho_n}{\rho}. \tag{72}$$

Equation (64) for temperature $T = T_\lambda$ yields relation $\rho_q(\rho)/\rho = f(\rho)$ and, hence, we have the following equation: $\alpha(\rho) \equiv f(\rho)$. Thus, Eqs. (35) and (65) and relation $\alpha(\rho) \equiv f(\rho)$ yield the function $\alpha(\rho)$ as

$$\alpha(\rho) = \left(\frac{M_q\epsilon}{2\pi\hbar^2}\right)^{3/2}\frac{M_q}{e^4\rho}\left[\frac{1}{4} - \left(\frac{\rho}{\rho_a}\right)^2 + \left(\frac{\rho}{\rho_a}\right)^4\right]^{3/2}, \tag{73}$$

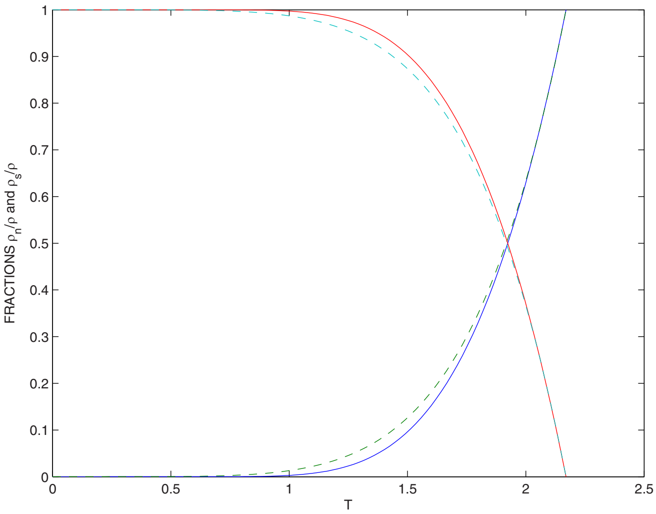

FIG. 1. Normal and superfluid fractions given by Eq. (74) (theory: solid line) and fit by Eq. (75) (experimental data: dashed line) for temperature region $T_p \leqslant T \leqslant T_\lambda$ and density $\rho = 0.145\ \mathrm{g\,cm^{-3}}$.

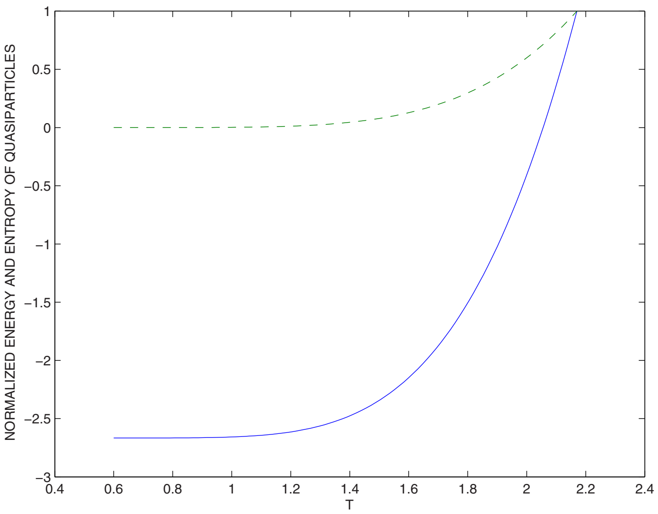

FIG. 2. Normalized energy (solid line) and entropy (dashed line) of diatomic quasiparticles given by Eqs. (68) and (69) for density $\rho = 0.145\ \mathrm{g\,cm^{-3}}$.

where $\rho_a = 6ma^3/\pi r_0^3$. Equations (63), (64), and (71) and relation $\alpha(\rho) \equiv f(\rho)$ lead to the normal and superfluid fractions,

$$\frac{\rho_n}{\rho} = \Phi(T,\rho), \quad \frac{\rho_s}{\rho} = [1 - \Phi(T,\rho)], \tag{74}$$

where the function $\Phi(T,\rho)$ is defined in Eq. (66).

The experimental data for the normal and superfluid fractions in liquid ^{4}He are well approximated for the range of temperatures $T_p \leqslant T \leqslant T_\lambda$ at saturated vapor pressure,

$$\frac{\rho_n}{\rho} = \left(\frac{T}{T_\lambda}\right)^{5.6}, \quad \frac{\rho_s}{\rho} = 1 - \left(\frac{T}{T_\lambda}\right)^{5.6}. \tag{75}$$

Theoretical normal and superfluid fractions given by Eq. (74) and experimental data approximated by Eq. (75) are shown in Fig. 1. In Fig. 2, we present the normalized energy and entropy of the diatomic quasiparticles given by Eqs. (68) and (69), respectively. In Fig. 3, we present the condensate fraction given by Eq. (63) (theory) and the fit of observed data for the condensate fraction by Glyde [46] which at SVP is $\rho_0/\rho = 0.0725[1 - (T/T_\lambda)^{5.5}]$. Thus, Figs. 1 and 3 demonstrate the good agreement of the theoretical results with experimental data for superfluid and BEC fractions at SVP in the range of temperatures $T_p \leqslant T \leqslant T_\lambda$.

VI. SUPERFLUID AND BEC FRACTIONS IN LIQUID ^{4}He FOR LOW TEMPERATURES

In the temperature interval $T \leqslant 0.5$ K, the most important excitations are the phonons. The phonon's energy is a linear function of the wave number k: $E_k = u_1 \hbar k$. This relation yields an equation for the free energy per unit volume as

$$\mathcal{F}(T,\rho) = \mathcal{F}_0(\rho) - \frac{\pi^2 k_B^4 T^4}{90\hbar^3 u_1^3}, \tag{76}$$

where u_1 is the first sound, $\mathcal{F}_0(\rho) = \mathcal{E}_0(\rho)\rho/m$, and $\mathcal{E}_0(\rho)$ is the ground-state energy per one particle at zero temperature.

The second sound in two-fluid hydrodynamics is given by

$$u_2 = \sqrt{\frac{\rho_s s^2}{\rho_n(\partial s/\partial T)_\rho}}, \tag{77}$$

where $s = \mathcal{S}/\rho$, and $\mathcal{S} = -\partial\mathcal{F}/\partial T$ is the entropy per unit volume. The entropy follows from Eq. (76) as

$$s = \Lambda T^3, \quad \Lambda = \frac{2\pi^2 k_B^4}{45\hbar^3 u_1^3 \rho}, \tag{78}$$

where the first sound u_1 does not depend on the temperature for the region, $T < 0.5$ K.

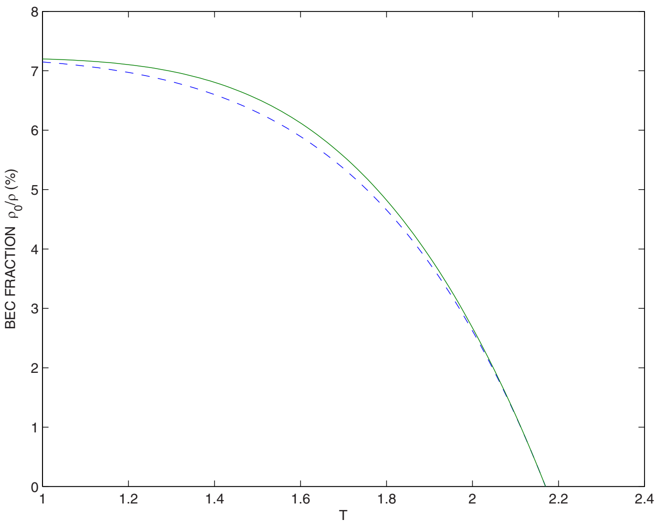

FIG. 3. Condensate fraction given by Eq. (63) (theory: solid line) and fit by Glyde [46] (experimental data: dashed line) for temperature region $T_p \leqslant T \leqslant T_\lambda$ ($\rho = 0.145\ \mathrm{g\,cm^{-3}}$).

We seek the normal and superfluid fractions for liquid ^{4}He at low temperatures $T \leqslant 0.5$ K in the form

$$\frac{\rho_n}{\rho} = \gamma(\rho)T^{\nu}, \quad \frac{\rho_s}{\rho} = 1 - \gamma(\rho)T^{\nu}. \tag{79}$$

Equations (76)–(79) yield the second sound as

$$u_2 = \sqrt{\frac{\Lambda}{3\gamma}(T^{4-\nu} - \gamma T^4)}. \tag{80}$$

There are only three different cases for parameter ν:

(1) $\nu < 4$, with $u_2 \to 0$ for $T \to 0$,
(2) $\nu > 4$, with $u_2 \to \infty$ for $T \to 0$,
(3) $\nu = 4$, with $u_2 \to \sqrt{\Lambda/3\gamma}$ for $T \to 0$.

We choose the case (3) with $\nu = 4$ because $u_2 \neq 0$ and $u_2 \neq \infty$ at zero temperature. Moreover, the limiting value for the second sound at $T \to 0$ is $u_2 = u_1/\sqrt{3}$ because the energy of the phonon excitations is a linear function of the wave number. It follows from Eq. (80) that the second sound for $T \leqslant 0.5$ K is

$$u_2 = \frac{u_1}{\sqrt{3}}[1 - \gamma(\rho)T^4]^{1/2}, \quad \gamma(\rho) = \frac{\Lambda}{u_1^2}. \tag{81}$$

The function $\gamma(\rho)$ is given by Eqs. (78) and (81) as

$$\gamma(\rho) = \frac{2\pi^2 k_B^4}{45\hbar^3 u_1^5 \rho}. \tag{82}$$

Equations (79) and (82) lead to normal and superfluid fractions of liquid ^{4}He for $T \leqslant 0.5$ K as

$$\frac{\rho_n}{\rho} = \left(\frac{2\pi^2 k_B^4}{45\hbar^3 u_1^5 \rho}\right)T^4, \quad \frac{\rho_s}{\rho} = 1 - \left(\frac{2\pi^2 k_B^4}{45\hbar^3 u_1^5 \rho}\right)T^4. \tag{83}$$

We can write the relation $\rho_0 = \alpha^*(\rho)\rho_s$ for temperature interval $T \leqslant 0.5$ K. In this case, $\rho = \rho_0 + \rho_{\text{ex}}$ and $\rho = \rho_s + \rho_n$ yield

$$\frac{\rho_0}{\rho} = \alpha^*(\rho)\frac{\rho_s}{\rho}, \quad \frac{\rho_{\text{ex}}}{\rho} = 1 - \alpha^*(\rho) + \alpha^*(\rho)\frac{\rho_n}{\rho}. \tag{84}$$

These equations are similar to Eqs. (71) and (72). However, the functions $\alpha(\rho)$ and $\alpha^*(\rho)$ are given for different temperature regions. Equations (83) and (84) yield, for zero temperature, the condensate fraction as $\rho_0/\rho = \alpha^*(\rho)$. The function $\alpha^*(\rho)$ can be found by Monte Carlo simulations of the condensate fraction in liquid ^{4}He at zero temperature. We choose the function $\alpha^*(\rho)$ in the form

$$\alpha^*(\rho) = C\exp(-\kappa_0\rho), \tag{85}$$

which is relevant to the Feynman approximation [51,52] for the ground-state wave function. However, such treatment leads to a rough estimate for the constants in Eq. (85). The data from Moroni *et al.* [35] lead to the constants in Eq. (85): $C = 6.05$ and $\kappa_0 = 30.6\ \text{cm}^3\,\text{g}^{-1}$.

The functions $\alpha(\rho)$ and $\alpha^*(\rho)$ given by Eqs. (73) and (85) are shown in Fig. 4. This figure demonstrates the difference between these functions. However, at low pressure, when the density is $\rho = 0.145\ \text{g}\,\text{cm}^{-3}$, we have the relation $\alpha(\rho) = \alpha^*(\rho)$. Equations (83) and (84) yield the condensate and excitation fractions as

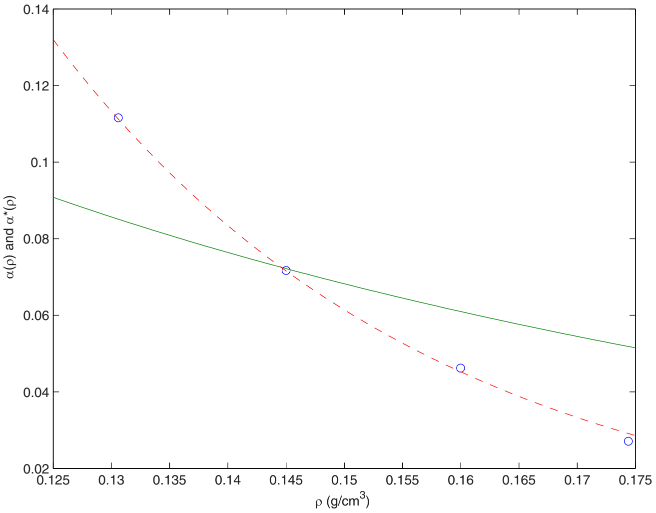

FIG. 4. Function $\alpha(\rho)$ given by Eq. (73) (solid line) for the region $T_p \leqslant T \leqslant T_\lambda$, and function $\alpha^*(\rho)$ given by Eq. (85) (dashed line) for temperature region $T \leqslant 0.5$ K. Condensate fraction in liquid ^{4}He for zero temperature from Ref. [35] (circles).

$$\frac{\rho_0}{\rho} = \alpha^*(\rho) - \left(\frac{2\pi^2 k_B^4 \alpha^*(\rho)}{45\hbar^3 u_1^5 \rho}\right)T^4, \tag{86}$$

$$\frac{\rho_{\text{ex}}}{\rho} = 1 - \alpha^*(\rho) + \left(\frac{2\pi^2 k_B^4 \alpha^*(\rho)}{45\hbar^3 u_1^5 \rho}\right)T^4. \tag{87}$$

Equation (86) for low temperature ($T \leqslant 0.5$ K) leads to the condensate fraction of liquid ^{4}He as $\rho_0/\rho = \alpha^*(\rho)$. It is also shown above that $\alpha(\rho) = \alpha^*(\rho)$ at SVP (see Fig. 4). Thus, the condensate fraction at low temperature and low pressure is $\rho_0/\rho = \alpha(\rho)$. We note that the function $\alpha(\rho)$ is found in Eq. (73) for the temperature region $T_p \leqslant T \leqslant T_\lambda$. However, the condensate fraction for the temperature region $0 \leqslant T \leqslant T_p$ ($T_p \simeq 1$ K) is a constant with a good accuracy. The fit of the observed data for the condensate fraction given by Glyde [46] at SVP ($\rho_0/\rho = 0.0725[1 - (T/T_\lambda)^{5.5}]$) shows that $\rho_0/\rho \simeq \text{const} = 0.0725$ for $T \leqslant T_p$. Hence, relation $\rho_0/\rho = \alpha(\rho)$ and Eq. (73) yield the condensate fraction for low temperature ($T \leqslant 0.5$ K) at SVP as $\rho_0/\rho = \alpha(\rho) = 7.22\%$.

Recent measurements show that for low temperatures at SVP, the condensate fraction is 7.25 ± 0.75% (see Ref. [46]), which is very close to our result (7.22%). The diffusion Monte Carlo simulations [35] for zero temperature give the condensate fraction as 7.17%. These results also agree for both Glyde *et al.* [30] and Snow *et al.* [53].

The developed theory also describes the bound temperature T_p as a function of density. Equations (74) and (83) with $T = T_p$ yield the equation for the bound temperature,

$$\Phi(T_p, \rho) = \gamma(\rho)T_p^4. \tag{88}$$

A simpler equation for the temperature T_p follows from Eqs. (75) and (83). We note that one can also use, in Eq. (75), the power $\nu = 11/2$, which does not violate the accuracy for the bound temperature T_p. In this case, we have following equation:

$$\left(\frac{T_p}{T_\lambda}\right)^{11/2}=\left(\frac{2\pi^2k_B^4}{45\hbar^3u_1^5\rho}\right)T_p^4, \tag{89}$$

which yields

$$T_p=\left(\frac{2\pi^2k_B^4T_\lambda^{11/2}}{45\hbar^3u_1^5\rho}\right)^{2/3}. \tag{90}$$

Hence, the bound temperature at SVP is $T_p \simeq 1$ K. This value also agrees with the experimental data presented in Refs. [45,54,55].

VII. CONCLUSIONS

In the present theory, the lambda transition temperature and Bose-Einstein condensation in liquid ^{4}He are described using the concept that for some temperature interval, there exist metastable diatomic clusters or diatomic quasiparticles which are the bound states of two atoms of ^{4}He. We emphasize that stable diatomic clusters or DQs can arise only in strong interacting Bose systems at high density and low temperatures. The DQs coupling in liquid ^{4}He for the temperatures below the lambda transition can be explained by the Lennard-Jones intermolecular potential. The ground-state energy E_0 of diatomic clusters or DQs for mass density $\rho = 0.145\ \mathrm{g\,cm^{-3}}$ is given by Eq. (19). This equation yields negative ground-state energy $E_0/k_B = -8.65$ K, which explains the existence of metastable clusters or DQs in liquid ^{4}He for low pressure and temperatures below the lambda transition temperature. The theory demonstrates that in liquid ^{4}He for the temperature region $1 \leqslant T \leqslant T_\lambda$ K, the diatomic quasiparticles macroscopically populate the ground state which leads to BEC in liquid ^{4}He. This approach yields the lambda transition temperature $T_\lambda = 2.16$ K, which is very close to the experimental λ temperature $T_\lambda = 2.17$ K. Figures 1 and 3 demonstrate the good agreement of theoretical superfluid and BEC fractions with experimental observations. It is shown (see Sec. VI) that the condensate fraction for low temperature ($T \leqslant 0.5$ K) at SVP is $\rho_0/\rho = \alpha(\rho) = 7.22\%$, which is very close to the value $7.25 \pm 0.75\%$ obtained in recent measurements (see Ref. [46]). The theory also demonstrates the connection between BEC and superfluidity phenomena in the temperature intervals $1 \leqslant T \leqslant T_\lambda$ K and $T \leqslant 0.5$ K by scaling laws given in Eqs. (71), (72), and (84). Thus, the diatomic quasiparticle concept leads to results which are in good agreement with experimental data at low pressure and the temperatures below the lambda transition temperature. The theory also demonstrates that BEC in dilute Bose gas and Bose fluid have a different nature. Indeed, the BEC in Bose fluid is connected with diatomic quasiparticles. However, DQs can arise only in strongly interacting Bose systems at high density and low temperatures.

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APPENDIX A: EFFECTIVE MASS OF DIATOMIC QUASIPARTICLES

In this Appendix, we present the renormalization procedure for the mass of diatomic quasiparticles in liquid ^{4}He for the temperature region $T_p \leqslant T \leqslant T_\lambda$. The energy of excited diatomic quasiparticles per unit volume follows from Eq. (60) as

$$\mathcal{U}_1=\frac{3}{2}k_BT\tilde{n}_1=\frac{3k_BT}{2\lambda_q^3(T)}\exp\left(-\frac{|E_0|}{k_BT}\right). \tag{A1}$$

The kinetic energy density of diatomic quasiparticles with the mass $M = 2m$ is given by

$$\mathcal{K}=\mathrm{Lim}\frac{1}{\mathrm{V}}\sum_{\mathbf{p}}\frac{\varepsilon(\mathbf{p})}{\exp\{\beta[\varepsilon(\mathbf{p})-\mu]\}-1}, \tag{A2}$$

where $\varepsilon(\mathbf{p}) = \mathbf{p}^2/2M$. The integration in this equation yields

$$\begin{aligned}\mathcal{K}&=\frac{1}{(2\pi\hbar)^3}\int\varepsilon(\mathbf{p})\exp\{-\beta[\varepsilon(\mathbf{p})-E_0]\}d\mathbf{p}\\&=\frac{3k_BT}{2\lambda^3(T)}\exp\left(-\frac{|E_0|}{k_BT}\right),\end{aligned} \tag{A3}$$

where $\lambda(T)$ is the thermal wavelength,

$$\lambda(T)=\left(\frac{2\pi\hbar^2}{Mk_BT}\right)^{1/2}. \tag{A4}$$

The energy density in Eq. (A1) can be written as $\mathcal{U}_1 = \mathcal{K} + \mathcal{V}$, where the potential energy density of the excited quasiparticles in harmonic approximation is given by $\mathcal{V} = \mathcal{K}$. Thus, we have, for the harmonic approximation, the relation

$$\mathcal{U}_1=2\mathcal{K}. \tag{A5}$$

The substitution of Eqs. (A1) and (A3) into Eq. (A5) yields

$$\frac{1}{\lambda_q^3(T)}=\frac{2}{\lambda^3(T)}, \tag{A6}$$

where the thermal wavelength $\lambda_q(T)$ is given in Eq. (56). Thus, Eq. (A6) leads to the effective (renormalized) mass,

$$M_q=\sigma M,\quad \sigma=2^{2/3}\simeq 1.587. \tag{A7}$$

Hence, the renormalized mass of the diatomic quasiparticles is given by $M_q = 2^{5/3}m$.

APPENDIX B: VIBRATIONAL MODES IN LIQUID ^{4}He

In this Appendix, we consider the energy of the vibrational modes of diatomic quasiparticles. The Hamiltonian for harmonic approximation is given by

$$\hat{H}_s=\frac{\hat{p}_s^2}{2M_q}+\frac{1}{2}M_q\omega_s^2\hat{x}_s^2, \tag{B1}$$

where $s = 1, 2, 3$. This Hamiltonian yields the following equation:

$$\frac{1}{2}M_q\omega_s^2\langle\hat{x}_s^2\rangle=\left\langle\frac{\hat{p}_s^2}{2M_q}\right\rangle, \tag{B2}$$

where the average kinetic energy is

$$\left\langle \frac{\hat{p}_s^2}{2M_q} \right\rangle = \frac{1}{2} k_B T. \tag{B3}$$

Equations (B2) and (B3) lead to relation

$$\frac{\hbar\omega_s}{k_B T} = \frac{\hbar}{\sqrt{M_q k_B T \langle \hat{x}_s^2 \rangle}}, \tag{B4}$$

where the effective mass is given by $M_q = 2^{5/3} m$ (see Appendix A). We accept that for mass density $\rho = 0.145\ \mathrm{g\,cm^{-3}}$, the relation $\sqrt{\langle \hat{x}_s^2 \rangle} \simeq 2d$ is approximately satisfied where $d \simeq 4.4 \times 10^{-8}$ cm is the average distance between helium atoms. In this case, Eq. (B4) for critical temperature T_c yields $\hbar\omega_s / k_B T_c \simeq 1/7$. Thus, we have found the inequality $\hbar\omega_s \ll k_B T_c$. This inequality also yields $\hbar\omega_k \ll |E_0|$ because the condition $|E_0| > k_B T_c$ is satisfied. The vibrational mode with $s = 0$ can be treated similarly.

APPENDIX C: THERMODYNAMICS OF DIATOMIC QUASIPARTICLES IN HELIUM FLUID

The partition function in Eq. (41) for the grand canonical density operator is given by

$$\ln \Xi_q = -\sum_{\mathbf{p}} \ln(1 - z_1 e^{-\beta \varepsilon_q(\mathbf{p})}) - \sum_{n_0} \sum_{n_1} \sum_{n_2} \sum_{n_3} \delta_{\{n\}} \ln(1 - z_0 e^{-\beta E_{\{n\}}}), \tag{C1}$$

where $z_k = \exp(\beta\mu_k)$ $(k = 0, 1)$. The change $V^{-1}\sum_{\mathbf{p}} \to (2\pi\hbar)^{-3} \int d\mathbf{p}$ (for the case $V \to \infty$) in Eq. (C1) yields

$$\frac{\ln \Xi_q}{V} = \frac{1}{\lambda_q^3} \zeta_{5/2}(z_1) - \frac{1}{V} \sum_{\{n\}} \delta_{\{n\}} \ln(1 - z_0 e^{-\beta E_{\{n\}}}), \tag{C2}$$

where $\zeta_s(z) \equiv \mathrm{Li}_s(z)$ is the polylogarithm (or generalized zeta function) and λ_q is the thermal wavelength,

$$\zeta_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s}, \quad \lambda_q = \left(\frac{2\pi\hbar^2\beta}{M_q} \right)^{1/2}. \tag{C3}$$

The density of the DQs for continuous and discrete energy spectra is

$$\frac{\tilde{N}_1}{V} = \frac{1}{\beta} \left[\frac{\partial}{\partial \mu_1} (V^{-1} \ln \Xi_q) \right]_{\mu_k = \tilde{\mu}} = \frac{1}{\lambda_q^3} \zeta_{3/2}(z), \tag{C4}$$

$$\frac{\tilde{N}_0}{V} = \frac{1}{\beta} \left[\frac{\partial}{\partial \mu_0} (V^{-1} \ln \Xi_q) \right]_{\mu_k = \tilde{\mu}} = \frac{1}{V} \sum_{\{n\}} \frac{\delta_{\{n\}}}{z^{-1} \exp(\beta E_{\{n\}}) - 1}, \tag{C5}$$

where $\mu_k = \tilde{\mu}$ $(k = 1, 2)$, $z = \exp(\beta\tilde{\mu})$, and chemical potential $\tilde{\mu}$ is given in Eq. (49). One can find that the condition $e^{-\beta|E_0|} \leqslant 0.0186$ is satisfied for $T \leqslant 2.17$ K because $E_0/k_B = -8.65$ K. Hence, the condition $e^{-\beta|E_0|} \ll 1$ is satisfied when $T \leqslant T_\lambda$. In this case, the polylogarithm in Eq. (C4) has decomposition as

$$\zeta_s(e^{-\beta|E_0|}) = e^{-\beta|E_0|} + 2^{-s} e^{-2\beta|E_0|} + \cdots, \tag{C6}$$

where the first term leads, with high accuracy, to function $\zeta_s(z)$. Thus, Eqs. (C4) and (C5) can be reduced to Eqs. (55) and (57) as

$$\tilde{n}_1 = \frac{1}{\lambda_q^3} \exp(-\beta|E_0|), \quad \tilde{n}_0 = \tilde{n}_q - \tilde{n}_1, \tag{C7}$$

where $\tilde{n}_1 = \mathrm{Lim}(\tilde{N}_1/V)$ and $\tilde{n}_0 = \mathrm{Lim}(\tilde{N}_0/V)$. The average energy of the DQs follows by Eqs. (40) and (41) as

$$U_q = \langle \hat{H}_q \rangle = -\left(\frac{\partial}{\partial \beta} \ln \Xi_q \right)_{\mu_k = \tilde{\mu}} + \tilde{\mu}\tilde{N}_0 + \tilde{\mu}\tilde{N}_1. \tag{C8}$$

The entropy of the diatomic quasiparticles in liquid ^{4}He is defined as $S_q = -k_B \{\mathrm{Tr}(\hat{\rho}_q \ln \hat{\rho}_q)\}_{\mu_k = \tilde{\mu}}$. It can be reduced by Eqs. (40) and (41) to the form

$$S_q = k_B \left(\ln \Xi_q - \beta \frac{\partial}{\partial \beta} \ln \Xi_q \right)_{\mu_k = \tilde{\mu}}, \tag{C9}$$

where the partition function Ξ_q is given in Eq. (C2).

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