Superfluid Bose Liquid with a Suppressed BEC and an Intensive Pair Coherent Condensate as a Model of ^{4}He

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One introduces a model of the superfluid state of a Bose liquid with repulsion between bosons, in which at $T = 0$, along with a weak single-particle Bose-Einstein condensate, there exists an intensive pair coherent condensate, analogous to the Cooper condensate in a Fermi liquid with attraction between fermions. A closed system of nonlinear integral equations for the normal and anomalous self-energy parts is solved numerically, and a quasiparticle spectrum is obtained, which is in good agreement with the experimental spectrum of elementary excitations in superfluid ^{4}He. It is shown that the roton minimum in the spectrum is associated with the negative minimum of the Fourier component of the pair interaction potential.

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Introduction.—Formulation of an *ab initio* theory of superfluidity (SF) of the ^{4}He Bose liquid is one of the most complex and important problems in quantum theory of many particles. Despite certain successes with modern computer methods (such as the Monte Carlo method [1] and the correlation basic function method [2] based on modern interatomic ^{4}He potentials [3–5]), the problem of an *ab initio* calculation of the quasiparticle spectrum (QPS) in the SF ^{4}He Bose liquid remains standing as well. Also, the microscopic field perturbation theory [6,7] calculation of the long-wave phonon part of the spectrum $E(p) \simeq c_1 p$, where c_1 is the speed of first sound, meets with difficulties—infrared divergencies and nonanalyticities at $p \to 0$ and $\epsilon \to 0$ [8–10].

On the other hand, according to numerous precise experimental data on neutron inelastic scattering [11–13] and to results in quantum evaporation of ^{4}He atoms [14], the maximal density ρ_0 of the single-particle Bose-Einstein condensate (BEC) in the ^{4}He Bose liquid even at very low temperatures $T \ll T_\lambda$ does not exceed 10% of the total density ρ of liquid ^{4}He, whereas the density of the SF component $\rho_s \to \rho$ at $T \to 0$. The fact that the BEC density is so low is implied by a strong interaction between ^{4}He atoms and means that the quantum structure of the SF condensate in He II with the "excess" density $(\rho_s - \rho_0) \gg \rho_0$ calls for a more thorough investigation.

In this paper, one discusses both the quantum structure of the SF state in a Bose liquid at $T = 0$ and the self-consistent calculation of the spectrum $E(p)$ of elementary excitations in the framework of renormalized field perturbation theory [8–10]. Our approach is based on the microscopic model [15] of superfluidity of a Bose liquid with a suppressed BEC and an intensive pair coherent condensate (PCC), which can arise from a sufficiently strong effective attraction between bosons in some domains of momentum space and is analogous to the Cooper condensate in a Fermi liquid with attraction between fermions near the Fermi surface [16]. As a small parameter, one uses the ratio of the BEC density to the total Bose liquid density $(n_0/n) \ll 1$, unlike in the Bogolyubov theory [17] for a quasi-ideal Bose gas, in which the small parameter is the ratio of the number of supracondensate excitations to the density of the intensive BEC, $(n - n_0)/n_0 \ll 1$. Because of this, the SF state within the model at hand can be described by a "short" self-consistent system of Dyson-Belyaev equations for the normal and anomalous self-energy parts $\tilde{\Sigma}_{ij}(\mathbf{k}, \omega)$ neglecting the diagrams of second and higher orders in the BEC density. Renormalized field perturbation theory [8–10] is used, which is built on combined field variables [9]. In this case, the SF component ρ_s is a superposition of the "weak" single-particle BEC and an intensive "Cooperlike" PCC with coinciding phases (signs) of the corresponding order parameters.

Choice of the pair interaction potential.—To describe interaction of helium atoms in real space, various semi-empirical potentials are conventionally used, all of which describe strong repulsion at small distances and weak van der Waals attraction at large distances [3–5]. However, those model potentials fail to take into account the fact that, at distances less than the quantum radius of the helium electron shell $r_0 = 1.22$ Å, the Coulomb repulsion between the nuclei $(Ze)^2/r$ (partially screened by bound electrons) sets in. The following simple approximation for the ^{4}He interatomic potential, diverging as r^{-1} at $r \to 0$, could be suggested:

$$V(r) = \begin{cases} \frac{4e^2}{r}(1 + \mu r)\exp(-r/\alpha), & r \le r_c, \\ \epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6], & r > r_c. \end{cases} \tag{1}$$

From the conditions of continuity of the potential $V(r)$ and its first derivative at $r = r_c$, one determines the values of parameters $r_c = 2.38$ Å and $\mu = 229$ Å^{-1} for $\alpha = r_0/2 = 0.61$ Å, $\epsilon = 10.8$ K, and $\sigma = 2.642$ Å. Such a potential has a finite Fourier component with an oscillating sign-changing momentum dependence (Fig. 1, dashed curve). The Fourier component will look alike for any potential of the form (1) in which the interaction at $r > r_c$ is determined by any of the modern ^{4}He potentials [3–5]. However, those Fourier components are analytically very complicated and technically very difficult to be used in the actual calculation. To be able to go forward while retaining the crucial features of the interaction, one should employ a model potential characterized by the same sign-changing Fourier component as the one of Eq. (1) but with a simpler analytic expression. We choose the simple finite repulsive potential of the "semitransparent spheres" model, $V(r) = (V_0/4\pi a^3)\theta(a-r)$ (θ is the step function), whose Fourier component

$$V(p) = V_0 \frac{\sin(pa) - pa\cos(pa)}{(pa)^3} \tag{2}$$

is an oscillating sign-changing function of momentum transfer p (Fig. 1, curve 1). It is to be emphasized that the existence of negative values of the Fourier component, $V(p) < 0$, is not directly associated with van der Waals forces, and the oscillations of said component arise even in the absence of attraction in real space, being an implication of quantum mechanical diffraction effects of mutual scattering of the particles.

The same behavior is characteristic of the Fourier component of more realistic potentials diverging not faster than r^{-2} at $r \to 0$ and possessing inflection points in the radial dependence.

The system of equations and the calculation of the quasiparticle spectrum in a Bose liquid with a suppressed BEC.—We use the system of Dyson-Belyaev equations [6], which allows one to express the normal $\tilde{G}_{11}$ and anomalous $\tilde{G}_{12}$ renormalized single-particle boson Green functions in terms of the respective self-energy parts $\tilde{\Sigma}_{11}$ and $\tilde{\Sigma}_{12}$ [8–10]. As was shown in Ref. [15], for a Bose liquid with strong enough interaction between particles, when the BEC is strongly suppressed, one can, when defining $\tilde{\Sigma}_{ik}(\mathbf{p}, \epsilon)$ in the form of a sequence of irreducible diagrams containing condensate lines, restrict oneself, with good precision, to the lowest terms in the expansion over the small BEC density ($n_0 \ll n$). As a result, up to terms of first order in the small parameter $n_0/n \ll 1$, for a Bose liquid one gets the "short" system of equations for $\tilde{\Sigma}_{ik}$:

$$\tilde{\Sigma}_{11}(\mathbf{p}, \epsilon) = n_0 \Lambda(\mathbf{p}, \epsilon)\tilde{V}(\mathbf{p}, \epsilon) + n_1 V(0) + \tilde{\Psi}_{11}(\mathbf{p}, \epsilon), \tag{3}$$

$$\tilde{\Sigma}_{12}(\mathbf{p}, \epsilon) = n_0 \Lambda(\mathbf{p}, \epsilon)\tilde{V}(\mathbf{p}, \epsilon) + \tilde{\Psi}_{12}(\mathbf{p}, \epsilon), \tag{4}$$

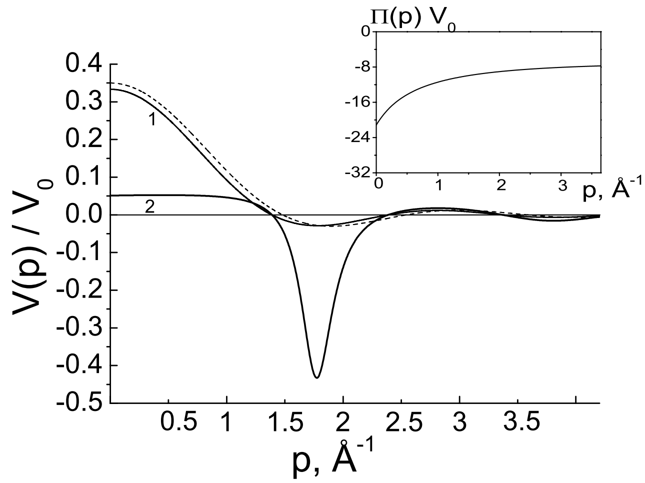

FIG. 1. The Fourier components of potential (1) (dashed curve); model potential (2) (curve 1); the corresponding renormalized potential (5), with account for the momentum dependence (6) of the polarization operator Π (inset) on the "mass shell" (curve 2).

where

$$\tilde{V}(\mathbf{p}, \epsilon) = V(p)[1 - V(p)\Pi(\mathbf{p}, \epsilon)]^{-1}. \tag{5}$$

Here $V(p)$ is the Fourier component of the input pair interaction potential; $\tilde{V}(\mathbf{p}, \epsilon)$ is the renormalized ("screened"), due to multiparticle collective effects, Fourier component of the nonlocal interaction; $\Pi(\mathbf{p}, \epsilon)$ is the boson polarization operator, accounting for the multiparticle collective effects:

$$\Pi(\mathbf{p}, \epsilon) = i \int \frac{d^3\mathbf{k}}{(2\pi)^3} \int \frac{d\omega}{2\pi} \Gamma(\mathbf{p}, \epsilon, \mathbf{k}, \omega) \times \{G_{11}(\mathbf{k}, \omega)G_{11}(\mathbf{k}+\mathbf{p}, \epsilon+\omega) + G_{12}(\mathbf{k}, \omega)G_{12}(\mathbf{k}+\mathbf{p}, \epsilon+\omega)\}. \tag{6}$$

$\Gamma(\mathbf{p}, \epsilon; \mathbf{k}, \omega)$ is the vertex part, which describes multiparticle correlations; $\Lambda(\mathbf{p}, \epsilon) = \Gamma(\mathbf{p}, \epsilon, 0, 0) = \Gamma(0, 0, \mathbf{p}, \epsilon)$, and n_1 is the number of supracondensate particles ($n_1 \gg n_0$), which is determined from the condition of conservation of the total number of particles. In the sequel, as well as in Ref. [15], we will take into account only the residues at the poles of single-particle Green functions $\tilde{G}_{ij}(\mathbf{p}, \epsilon)$, neglecting the contributions of eventual poles of the functions $\Gamma(\mathbf{p}, \epsilon, \mathbf{k}, \omega)$ and $\tilde{V}(\mathbf{p}, \epsilon)$, which do not coincide with the poles of $\tilde{G}_{ij}(\mathbf{p}, \epsilon)$. As a result, the functions $\tilde{\Psi}_{ij}(\mathbf{p}, \epsilon)$ on the "mass shell" $\epsilon = E(p)$ assume the following form (at $T = 0$):

$$\tilde{\Psi}_{11}[\mathbf{p}, E(p)] = \frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \Gamma[\mathbf{p}, E(p); \mathbf{k}, E(k)] \tilde{V}[\mathbf{p}-\mathbf{k}, E(p)-E(k)] \left[\frac{A[k, E(k)]}{E(k)} - 1\right], \tag{7}$$

$$\tilde{\Psi}_{12}[\mathbf{p}, E(p)] = -\frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{V}[\mathbf{p}-\mathbf{k}, E(p)-E(k)] \Gamma[\mathbf{p}, E(p); \mathbf{k}, E(k)] \frac{n_0 \Lambda[\mathbf{k}, E(k)]\tilde{V}[\mathbf{k}, E(k)] + \tilde{\Psi}_{12}[\mathbf{k}, E(k)]}{E(k)}, \tag{8}$$

where

$$E(p) = \frac{1}{2}\{\tilde{\Psi}_{11}[\mathbf{p}, E(p)] - \tilde{\Psi}_{11}[-\mathbf{p}, -E(p)]\} + \{A^2[\mathbf{p}, E(p)] - \{n_0\Lambda[\mathbf{p}, E(p)]\tilde{V}[\mathbf{p}, E(p)] + \tilde{\Psi}_{12}[\mathbf{p}, E(p)]\}^2\}^{1/2}, \quad (9)$$

$$A[\mathbf{p}, E(p)] = n_0\Lambda[\mathbf{p}, E(p)]\tilde{V}[\mathbf{p}, E(p)] + \tilde{\Psi}_{12}(0,0) - \tilde{\Psi}_{11}(0,0) + \frac{1}{2}\{\tilde{\Psi}_{11}[\mathbf{p}, E(p)] + \tilde{\Psi}_{11}[-\mathbf{p}, -E(p)]\} + \frac{p^2}{2m}. \quad (10)$$

In this case, the total quasiparticle concentration is determined by the relation

$$n = n_0 + \frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\left[\frac{A[\mathbf{k}, E(k)]}{E(k)} - 1\right]. \quad (11)$$

From Eqs. (9) and (10), it follows that the QPS, because of the analyticity of the functions $\tilde{\Psi}_{ij}(\mathbf{p}, \epsilon)$, is acoustic at $p \to 0$, and its structure at $p \neq 0$ depends essentially on the character of the renormalized pair interaction of bosons.

Note that in the absence of a BEC ($n_0 = 0$), Eq. (8) becomes homogeneous and degenerate with respect to the phase of the function $\tilde{\Psi}_{12}(\mathbf{p})$. It is then analogous to the Bethe-Goldstone equation for a pair of particles in momentum space $\Psi(\mathbf{p}) = -\int \frac{d^3\mathbf{k}}{(2\pi)^3} V(\mathbf{p} - \mathbf{k}) \frac{\Psi(\mathbf{k})}{2E(k) - \Omega}$, with zero binding energy $\Omega = 0$, which has a nontrivial solution only in the case of attraction $V(q) < 0$. This analogy allows one to treat $\tilde{\Psi}_{12}(\mathbf{p})$ at $n_0 = 0$ as a PCC order parameter [15], which describes boson pair condensation in momentum space (identical to the Cooper condensate of fermion pairs [16]). Equation (8) being degenerate over the phase of $\tilde{\Psi}_{12}(\mathbf{p})$ at $n_0 \to 0$ allows one to meet the condition of stability of the phonon spectrum $c_1^2 = \tilde{\Psi}_{12}(0)/\tilde{m}^* > 0$ by choosing the appropriate sign of the pair order parameter $\tilde{\Psi}_{12}(0) > 0$. Since at $T = 0$ the density ρ_s of the SF component, on the one hand, coincides with the total density $\rho = mn$ of the Bose liquid and, on the other hand, is proportional to $\tilde{\Sigma}_{12}(0)$, which plays the role of the SF order parameter, one gets the following relations:

$$\rho_s \equiv \rho_0 + \tilde{\rho}_s = \beta m \frac{\tilde{\Sigma}_{12}(0)}{\Lambda(0)\tilde{V}(0)} = \beta m[n_0(1 - \gamma) + \Psi], \quad (12)$$

where

$$\gamma \equiv \frac{1}{(2\pi)^2\Lambda(0)\tilde{V}(0)}\int_0^\infty \frac{k^2 dk}{E(k)}[\Lambda(k)\tilde{V}(k)]^2, \quad (13)$$

$$\Psi \equiv -\frac{1}{(2\pi)^2\Lambda(0)\tilde{V}(0)}\int_0^\infty \frac{k^2 dk}{E(k)}\Lambda(k)\tilde{V}(k)\tilde{\Psi}_{12}(k), \quad (14)$$

and β is a certain dimensionless constant. Since the density of the single-particle BEC is equal to $\rho_0 = mn_0$, we obtain $\beta = (1 - \gamma)^{-1}$. This means that the density of the Cooperlike PCC is

$$\tilde{\rho}_s = mn_1 = \frac{m\Psi}{(1 - \gamma)}, \quad (15)$$

the concentration $n_1 = n - n_0$ being then determined from relation (11), and for liquid ^{4}He at $T \to 0$, in accordance with the experimental data [11–14], it should be approximately 90% of the full concentration $n = 2.17 \times 10^{22}$ cm^{-3}. Thus, the SF component of the Bose liquid at $T = 0$ in this model is an effective coherent condensate [10] which is a superposition of the weak one-particle BEC and the intensive PCC.

The key point in the behavior of the Fourier component of the screened potential $\tilde{V}[\mathbf{p}, E(p)]$ is that, as long as the quasiparticle spectrum $E(p)$ satisfies the condition of stability with respect to decay into a pair of quasiparticles, $E(p) < E(k) + E(p - k)$, the real part of the polarization operator is negative: $\Re\Pi[\mathbf{p}, E(p)] < 0$ on the "mass shell" (Fig. 1, inset). As a result, both the strong suppression of repulsion in the region where $V(p) > 0$ and strong enhancement of attraction in the region where $V(p) < 0$ take place (compare curves 1 and 2 of Fig. 1).

In order to calculate the QPS $E(p)$, one has computed the polarization operator (6) and the renormalized retarded interaction (5) on the "mass shell" $\omega = E(p)$ as well as for $\omega = E(p) \pm E(k)$, while at the same time solving the nonlinear integral equations (7) and (8) for the functions $\tilde{\Psi}_{ij}[\mathbf{p}, \pm E(p)]$. The only parameter, varied in order to ensure the best coincidence of $E(p)$ with the empirical ^{4}He QPS $E_{\text{exp}}(p)$, was the amplitude V_0 of the initial potential (2) (we have taken $V_0/a^3 = 1552$ K at $a = 2.44$ Å). The BEC concentration was given, in accordance with the experimental data [14], as $n_0 = 9\%n = 1.95 \times 10^{21}$ cm^{-3}. Figure 1, curve 2, depicts the momentum dependence of the renormalized retarded interaction (5) obtained. In Fig. 2, the solid line is the theoretical QPS $E(p)$ (9), the dots are the experimental spectrum [19–22], as are the asterisks, beyond the roton minimum ($T = 0.6$ K) [18]. Note that the phase velocity of quasiparticles $[E(p)/p]|_{p\to 0}$ obtained within this model coincides with the speed of hydrodynamic sound $c_1 \simeq 236$ m/s in liquid ^{4}He. Satisfactory agreement of $E(p)$ with $E_{\text{exp}}(p)$ at $p \leq 3.5$ Å^{-1} is evident.

One has constructed a self-consistent microscopic theory of the SF Bose liquid and carried out an *ab initio* calculation of the QPS $E(p)$. The pair attraction of bosons in certain regions of momentum space, enhanced because

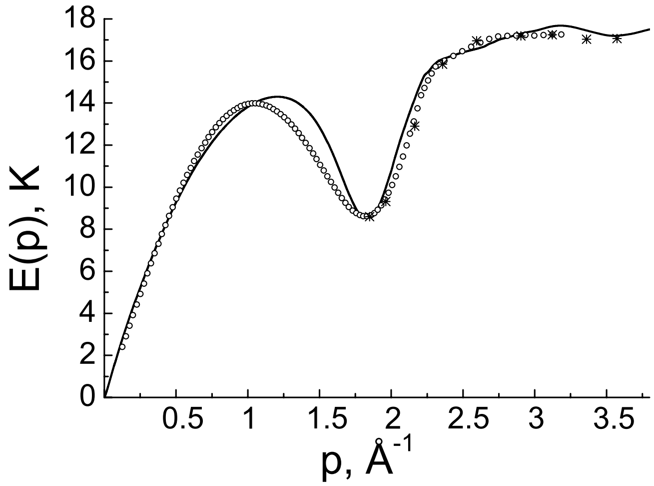

FIG. 2. The theoretical quasiparticle spectrum $E(p)$ obtained by a self-consistent calculation (solid line); the empirical ^{4}He excitation spectrum (circles); the spectrum beyond the roton minimum, Ref. [22] (asterisks).

$\Re\Pi(\mathbf{p}, \omega) < 0$ on the "mass shell," leads to formation of an intensive PCC, which, together with a weak BEC, forms a unified coherent condensate. Such condensate is the microscopic foundation of the SF component of the Bose liquid. The self-consistency of the model is confirmed by that, on the one hand, the theoretical value of the full particle density from Eq. (11), $n_{\text{th}} = 2.14 \times 10^{22}\ \text{cm}^{-3}$, is close to the experimental ^{4}He density; on the other hand, the density n_1 of supracondensate particles from Eq. (15) for the values of parameters indicated is above 90%n, which also agrees with experiment, taking into account that the BEC density is determined to be up to about 10%n. The main result of this model of the SF state of a Bose liquid with a suppressed BEC and with an intensive PCC is the conclusion that the roton minimum in the spectrum $E(p)$ and, accordingly, the maximum in the structure factor $S[p, E(p)]$ is associated with the first negative minimum of the Fourier component of the renormalized (screened) interaction potential. A good agreement of the theoretical QPS with $E_{\text{exp}}(p)$ is obtained with only one variational parameter being used—the amplitude V_0 of the initial model potential.

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