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A.S.Shumovsky, V.I.Yukalov

MICROSCOPIC MODEL FOR SUPERCONDUCTOR WITH NORMAL STATE NUCLEI

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The representation of a superconductor as the equilibrium mixture of two electron liquids is the basis of the phenomenological theories developed by Gorter and Casimir, F.London and H.London, Ginsburg and Landau (see ref. [1]). It is supposed in these theories that the total free energy of a system in the superconducting phase has a form

$$F(w,\Theta) = f(1-w)F_n(\Theta) + \phi(w)F_s(\Theta),$$

where $F_i(\Theta)$ is the free energy for normal or superconducting electrons and $f(\cdot),\phi(\cdot)$ are some functions of the superconducting electron concentration w. The form of these functions is determined from the comparison with the experimental data.

In a microscopic theory superconductor is described by an effective four-fermion Hamiltonian [2,3] which is gauge invariant [4] with the symmetry group U(1). However, the superconducting state is not gauge invariant. So, in compliance with the quasi-means method of Bogolubov [4,5] it can be described as follows. Due to the transformation

$$\overset{+}{a}(k,\uparrow)\,\overset{+}{a}(-k,\downarrow) = \sigma^-(k),\quad a(-k,\downarrow)\,a(k,\uparrow) = \sigma^+(k),\quad \sigma^{\pm}(k) = \{\sigma^x(k) \pm i\sigma^y(k)\}/2,$$

the quasi-spin representation can be constructed [6]. Here σ^α is a component of Pauli spin vector and $a^+(\cdot), a(\cdot)$ are the fermi-operators for electrons. Let ϕ be the polar angle in the XY-plane of quasi-spin space. The Bogolubov-BCS Hamiltonian is invariant with respect to the gauge transformation $a(k) \to a(k)\,e^{i\phi/2}$ [5] which describes the rotation of k-th quasi-spin. The k-th quasi-spin state $\psi_{k\phi}$ with the angle ϕ obeys the condition [7]

$$(\vec{\sigma}(k)\cdot\vec{E}_\phi)\,\psi_{k\phi} = \psi_{k\phi},$$

where $\vec{E}_\phi$ is the three-dimensional vector with the polar angle ϕ for the projection on the XY-plane. The vacuum state of the whole system, characterised by the angle ϕ, is

$$\psi_\phi = \prod_k \otimes \psi_{\phi k},\quad \psi_\phi \in \mathcal{H}_\phi.$$

Here $\mathcal{H}_\phi$ is the incomplete Neumann product of two-dimensional "one-particle" Hilbert spaces [7]. One can easily see that two states $\psi_\phi, \psi_{\phi'}\ (\phi \neq \phi', -\phi')$ are orthogonal to each other in the thermodynamic limit. Let us fix the angle $\phi=0$. The states $\psi_0 \in \mathcal{H}_0$ are noninvariant with respect to U(1) group. So, they can describe the "superconducting electrons" $(\mathcal{H}_0 \equiv \mathcal{H}^{(s)})$.

Alternatively, the space $\mathcal{H}^{(n)}$

$$\forall\phi \quad \mathcal{H}^{(n)} \neq \mathcal{H}_\phi$$

contains the invariant states with respect to U(1). In the framework of the quasi-means method each phase state of the system is defined on the corresponding space of states.

It is natural to define the two-liquid mixture on the space [8]

$$\mathcal{H} = \mathcal{H}^{(n)} \otimes \mathcal{H}^{(s)}.$$

In this case the total Hamiltonian of the system H, which is constructed from the operators $\overset{+}{a}, a$, should be defined as a direct sum of the suitable nonequivalent representations

$$H = H_n \oplus H_s.$$

Now we shall use the approach of the papers [9,10], which was developed for the description of the heterophase states. At first it should be noted that the existence of equilibrium states in statistical mechanics is stipulated by the limit of $t \to +\infty$, where t is the time of observation. In a uniform system the heterophase fluctuations can freely move in the whole volume of the system and their sizes and number can change. The complete uniform mixing should be performed in the macroscopic system at $t \to +\infty$. Then, any point of the volume can contain the electron corresponding to the definite phase (with the state on $\mathcal{H}_i$) with the suitable probability. For such a phase mixture the existence of an electron with momentum k and spin s and its phase quality are the independent events. So, it is natural to renorm the operators by the following manner [8]

$$a_i(\cdot) \to \sqrt{w_i}\,\tilde{a}_i(\cdot),$$

where the phase concentration w_i is defined by the condition

$$w_i = \frac{N_i}{N},\quad N \equiv \sum_i N_i,\quad N_i = \sum_{k,s} \langle \overset{+}{a}_i(k,s)\,a_i(k,s)\rangle,\quad (i = n,s). \qquad (1)$$

The same method was used for the construction of the microscopic model of a ferromagnet with paramagnetic nuclei [11,12]. Let us consider for generality the Hamiltonian containing an effective attraction and Coulomb repulsion of electrons as well

$$H = H_n \oplus H_s, \qquad H_i = w_i T_i - w_i^2(A_i - Q_i). \qquad (2)$$

Here

$$T_i^s \equiv \sum_k \epsilon_i(k)\,n_i(k),\quad \epsilon_i(k) = \frac{k^2}{2m} - \mu_i,\quad n_i(k) \equiv \sum_s \overset{+}{\tilde{a}}_i(k,s)\,\tilde{a}_i(k,s);$$

$$A_i \equiv \frac{1}{2V} \sum_{kk'} J(k,k') \tilde{a}^{+}_i(k,\uparrow) \tilde{a}^{+}_i(-k,\downarrow) \tilde{a}_i(-k',\downarrow) \tilde{a}_i(k',\uparrow);$$

$$Q_i \equiv \frac{1}{2V} \sum_{\substack{q \\ (q \neq 0)}} U(q) \rho^{+}_i(q) \rho_i(q), \quad U(q) = \frac{4\pi e^2}{|q|^2}, \quad \rho_i(q) = \sum_{k,s} \tilde{a}^{+}_i(k+q,s) \tilde{a}_i(k,s)$$

Here μ_i is the chemical potential of i -th phase, $J(\cdot)$ is the parameter of the effective interaction and $\rho(q)$ is the Fourier-components of the space density of electrons. Then in compliance with expressions

$$N_i = -\frac{\partial \Omega_i}{\partial \mu_i}, \quad \Omega_i = -\Theta \ln \mathrm{Sp}\, e^{-H_i/\Theta}$$

(Θ is the temperature) the normalization condition (1) can be presented in a form of

$$w_s = \frac{w_s \sum_k \langle n_s(k) \rangle}{\sum_k [w_s \langle n_s(k) \rangle - (1-w_s) \langle n_n(k) \rangle]}, \quad w_n = 1 - w_s. \tag{3}$$

Besides that we have the phase equilibrium condition $\mu_n = \mu_s$ which has the form

$$\frac{\partial F_n}{\partial w_n} = \frac{\partial F_s}{\partial w_s}, \quad F_i = \Omega_i + \mu_i w_i N.$$

Thus we obtain

$$2 w_s \sum_i \langle Q_i - A_i \rangle = \langle T_n - T_s \rangle + 2 \langle Q_n - A_n \rangle. \tag{4}$$

Here $\langle X_i \rangle$ denotes the mean value of the operator X_i. One can define w_s, w_n and μ from the equations (3), (4) as functions of Θ and of interaction parameters.

The two-liquid model of a superconductor is completely described by the expressions (2)-(4). It should be emphasized that for the special case of $w_s \equiv 1$, which is a possible solution of eq. (3), and when $Q = 0$ the Hamiltonian (2) coincides with the standard Bogolubov-BCS model.

Let us consider some general properties of the model problem (2)-(4). One can easily see from (3) that $w_s = 0$ is one of the possible solutions. It is known that such solution is not stable below the critical point Θ_c. In this point the macroscopic distinction between the phase components disappears. So, from (3), (4) we have

$$w_s(\Theta_c) = w_n(\Theta_c) = 1/2.$$

It should be noted that in the phenomenological theories [1] $w_s(\Theta_c) = 0$, $w_n(\Theta_c) = 1$. Below the critical point the concentration w_s increases with decreasing temperature and reaches the value $w_s = 1$ at the nucleation point which obeys the condition

$$2 \langle Q_s(\Theta_N) - A_s(\Theta_N) \rangle = \langle T_n(\Theta_N) - T_s(\Theta_N) \rangle. \tag{5}$$

Below the nucleation point Θ_N there is the pure superconducting state in the system ($w_s \equiv 1$, $\Theta \leq \Theta_N$). In the nucleation point there exists a discontinuity for the derivative of the order parameter $\Delta = \frac{1}{V} \sum_k J(k,k') \langle \tilde{a}^{+}_i(k',\uparrow) \tilde{a}^{+}_i(-k',\downarrow) \rangle$ and apparently there is a jump of the specific heat. It should be outlined that $\Theta_N = 0$ in the phenomenological theories. In the model under consideration the case of $\Theta_N > 0$ can obey the equation (5) for some definite values of the parametrs of the effective and Coulomb interactions. Moreover, for the large $\langle Q_s \rangle$ the equation (5) has apparently no solution $\Theta_N \geq 0$, i.e., the ground state of the system is not purely superconducting and it contains the microscopic quota of normal electrons. The deflection of w_s at $\Theta = 0$ from unity should change the character of the electron-density fine distribution that could be observed by the experimental way [13]. Besides this, such system has to obtain some residual resistance and residual heat conductivity.

Let us now consider the simple case of $Q \to 0$ (the exclusion of the Coulomb interaction). When $Q = 0$ a rigorous calculation of $\langle T_i \rangle$ and $\langle A_i \rangle$ can be done in the framework of the Trial Hamiltonian Method [14]. We suppose now that [15]

$$J(k,k') = \begin{cases} J = \mathrm{const}, & |\epsilon(k)| \leq \hbar\omega_0 \\ 0, & |\epsilon(k)| > \hbar\omega_0. \end{cases}$$

It can be easily seen that in this case the phase transition into the stable state with $w_s \equiv 1$ (at $\Theta \leq \Theta_c$) occurs in the point

$$\Theta_c = 1,134\, e^{-1/\rho_0 J},$$

which conforms with the Bogolubov-BCS critical point. Here ρ_0 is the density of states per unit volume and per unit energy on the Fermi surface. Besides the stable state a metastable one can arise at $\Theta \leq \tilde{\Theta}_c$, where

$$\tilde{\Theta}_c = 0.567\, e^{-2/\rho_0 J} = \frac{1}{2} \Theta_c e^{-1/\rho_0 J}.$$

The concentration $w_s = \frac{1}{2}$ in the point $\tilde{\Theta}_c$; and below $\tilde{\Theta}_c$ the value of w_s increases with the decrease of temperature up to the value $w_s = 1$ at $\Theta = 0$.

So the stable two-liquid state is impossible when the Coulomb interaction is absent in the system. Thus, we arrive

at conclusion that the existence of the normal component below the critical point in the superconductor is due to the competition between the effective attraction and the Coulomb repulsion of electrons.

The detailed quantitative examination of the microscopic two-liquid model for the superconductor which is constructed in the present paper can be produced by the known methods [3,14,15]. The consideration of the external magnetic field is also interesting because it plays the role of the suplement disordering factor. It has a special importance for the case of hard superconductors. We intend to perform this program in the other papers.

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