THERMODYNAMIC PROPERTIES OF SUPERCONDUCTORS WITH A NONMAGNETIC IMPURITY.

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Abstract

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THERMODYNAMIC PROPERTIES OF SUPERCONDUCTORS WITH A NONMAGNETIC IMPURITY.

ALLOWANCE FOR THE OVERLAP OF ENERGY BANDS

(Presented by Academician N. N. Bogolyubov, 12 XII 1966)

The theory of superconductors with overlapping energy bands in the vicinity of the Fermi energy was considered in works ([1–5]). On the basis of the results obtained in these works, we shall consider the thermodynamic properties of a two-band model of a superconductor with small amounts of a nonmagnetic impurity. We shall investigate the nature of the change in the order parameters with increasing impurity concentration, determine the energy gap in the spectrum of Fermi elementary excitations, and calculate the electronic heat capacity. The calculations will be carried out in the limiting cases of temperatures close to the critical temperature (T_c) and to zero temperature. The notation is the same as in works ([3–5]).

Let us denote by G_n, P_n, and R_n the temperature Green' s functions of the n-th band of a superconductor with an impurity (after averaging over the positions of the latter). Then one may write:

$$\overline{G}_n(\mathbf{k}|\Omega) = [i\Omega + \varepsilon_n(\mathbf{k}) - \overline{\sigma}_n(-\mathbf{k}| - \Omega)]/A_n(\mathbf{k}|\Omega),$$
$$\overline{P}_n(\mathbf{k}|\Omega) = [\Gamma_n + \overline{\Sigma}_n(\mathbf{k}|\Omega)]^*/A_n(\mathbf{k}|\Omega), \quad (1)$$
$$A_n(\mathbf{k}|\Omega) = [\varepsilon_n(\mathbf{k}) + i\Omega - \overline{\sigma}_n(-\mathbf{k}| - \Omega)][\varepsilon_n(\mathbf{k}) - i\Omega - \overline{\sigma}_n(\mathbf{k}|\Omega)] + |\Gamma_n + \overline{\Sigma}_n(\mathbf{k}|\Omega)|^2,$$

where

$$\Gamma_n^* = \sum_m V_{mn} \frac{1}{\beta V} \sum_{\mathbf{k}\Omega} \overline{P}_m(\mathbf{k}|\Omega); \quad (2)$$

V_{mn} are the constants of the effective electron-electron interaction of the two-band model (on the Fermi surface). The function $\overline{R}_n$, not written out, is the

complex conjugate of the function $\overline{P}_n$. The contribution of the impurity interaction to the mass operators σ_n and Σ_n has the form:

$$\overline{\sigma}_n(\mathbf{k}|\Omega) = \frac{c}{V}\sum_m \sum_{\mathbf{k}'} |u(\mathbf{k}-\mathbf{k}')|^2 \overline{G}_m(\mathbf{k}'|\Omega)|\chi(n\mathbf{k}, m\mathbf{k}')|^2,$$
$$\overline{\Sigma}_n(\mathbf{k}|\Omega) = \frac{c}{V}\sum_m \sum_{\mathbf{k}'} |u(\mathbf{k}-\mathbf{k}')|^2 \overline{R}_m(\mathbf{k}'|\Omega)|\chi(n\mathbf{k}, m\mathbf{k}')|^2, \tag{3}$$

where $\chi(n\mathbf{k}, m\mathbf{k}')$ is the integral over the unit cell of the modulating factors $u_{n\mathbf{k}}$ and $u_{m\mathbf{k}'}$ of the Bloch functions of the electrons in the metal.

Taking into account that the principal values of the Green' s functions are concentrated near the bands of the Fermi surface (we assume them to be spherical), with radii k_n^F and k_m^F, we solve equations (1)–(3) in the following way:

$$\overline{\sigma}_n(\mathbf{k}|\Omega) \simeq i\Omega t_n(\Omega); \qquad \overline{\Sigma}_n(\mathbf{k}|\Omega) \simeq \Gamma_n X_n(\Omega), \tag{4}$$
$$t_n(\Omega) = \sum_m \frac{\hbar}{2\tau_{nm}|\Omega|}\frac{u_m}{\sqrt{u_m^2+1}},$$
$$\Gamma_n X_n(\Omega) = \sum_m \frac{\hbar}{2\tau_{nm}}\frac{1}{\sqrt{u_m^2+1}}, \qquad u_m = \frac{|\Omega|}{\Gamma_m}\frac{1+t_m}{1+X_m},$$

where in the two-zone case we have

$$u_1 + \alpha_1(u_1-u_2)/\sqrt{u_2^2+1} = |\Omega|/\Gamma_1, \qquad \alpha_1 = \hbar/2\tau_{12}\Gamma_1,$$
$$u_2 + \alpha_2(u_2-u_1)/\sqrt{u_1^2+1} = |\Omega|/\Gamma_2, \qquad \alpha_2 = \hbar/2\tau_{21}\Gamma_2. \tag{5}$$

On the basis of these formulas, for the order parameters Γ_n we obtain the equations

$$\Gamma_n = \sum_m V_{mn}N_m\frac{\pi}{\beta}\sum_\Omega \frac{1}{\sqrt{u_m^2+1}}. \tag{6}$$

Let us now proceed to the investigation of the order parameters at zero temperature.

Although the impurity concentration considered by us does not exceed several percent, we can distinguish two limiting cases: a low impurity concentration ($\alpha_i \ll 1$) and a high impurity concentration ($\alpha_i \gg 1$). The solution of equations (6) in the first case differs from the values of the gaps γ_n of the pure substance by small corrections:

$$\Gamma_n = \gamma_n + \gamma_n', \tag{7}$$

where

$$\begin{aligned}\gamma_1' = \frac{\hbar}{2\tau_{12}}\left[\frac{2\gamma_2}{\gamma_1+\gamma_2}K\left[\frac{|\gamma_1-\gamma_2|}{\gamma_1+\gamma_2}\right]-E\left[\frac{|\gamma_1-\gamma_2|}{\gamma_1+\gamma_2}\right]\right]\left(1-\frac{V_{21}N_2\gamma_2}{d\gamma_1}\right)\\ +\frac{V_{21}N_2}{d}\frac{\hbar}{2\tau_{21}}\left[\frac{2\gamma_1}{\gamma_1+\gamma_2}K\left[\frac{|\gamma_1-\gamma_2|}{\gamma_1+\gamma_2}\right]-E\left[\frac{|\gamma_1-\gamma_2|}{\gamma_1+\gamma_2}\right]\right],\end{aligned} \tag{8}$$

$$d = a + N_1V_{12}\gamma_1/\gamma_2 + N_2V_{21}\gamma_2/\gamma_1, \qquad a = N_1N_2(V_{11}V_{22}-V_{12}V_{21}).$$

K, E are complete elliptic integrals. The quantity γ_2' is obtained from γ_1' by replacing the index $1 \rightleftarrows 2$. Both of these quantities are negative, i.e., the impurity reduces the order parameters. In the case of a high impurity concentration ($\alpha_i \gg 1$) we obtain the following results:

$$\gamma_1/\Gamma_1 = \gamma_2/\Gamma_2,$$

$$\ln\left[\frac{\gamma_1}{\Gamma_1}\frac{\sqrt{z}\,(N_1+N_2)}{(N_2+N_1z)}\right] = -\frac{N_1N_2(1-z)^2}{(N_2+N_1z)^2}\ln\left[2\sqrt{z}\,\bar{\alpha}_1\left(1+\frac{N_1}{N_2}\right)\right]+\frac{(N_1+N_2)(N_2-N_1z^2)}{2(N_2+N_1z)^2}\ln z, \tag{9}$$

where

$$z = \gamma_1/\gamma_2, \qquad \bar{\alpha}_1 = \hbar/2\tau_{12}\gamma_1, \qquad \bar{\alpha}_2/\bar{\alpha}_1 = (N_1/N_2)z. \tag{10}$$

Thus, in this limiting case the ratio γ_1/Γ_1 increases with increasing impurity concentration according to a power law, i.e., a further decrease of the quantity Γ_n occurs. In the concentration range considered by us, the order parameters do not, generally speaking, become zero and, consequently, the superconducting state of the metal is preserved.

Let us calculate the density of states $\mathcal{N}_n(\Omega)$ in this temperature region. This quantity is defined as follows:

$$\mathcal{N}_n(\Omega) = N_n\,\mathrm{Re}\left[u_n/\sqrt{u_n^2-1}\right], \tag{11}$$

where in the present case the quantities u_n and the frequency Ω are related by the equations

$$\Omega/\Gamma_1 = u_1 + i\alpha_1(u_1 - u_2)/\sqrt{u_2^2 - 1}, \qquad \Omega/\Gamma_2 = u_2 + i\alpha_2(u_2 - u_1)/\sqrt{u_1^2 - 1}, \tag{12}$$

which are obtained from (5) by the replacement (6)

$$u_n \to -iu_n, \qquad \Omega \to i\Omega, \qquad \Gamma_n \to \Gamma_n.$$

It can be shown that when one of the two densities $\mathcal{N}_n$ is equal to zero, the other density is also equal to zero. Both densities begin to take on nonzero values at a certain frequency Ω_0, which, according to ([6],[7]), plays the role of a gap in the electronic energy spectrum. At a high impurity concentration ($a_i \gg 1$), the energy gap has the form

$$\Omega_0 = \Gamma_1\Gamma_2(a_1 + a_2)/(a_1\Gamma_1 + a_2\Gamma_2). \tag{13}$$

It follows from this that the quantity Ω_0 is greater than the smaller of the two order parameters Γ_n and smaller than the larger of them. Since, as was shown, the Γ_n decrease with increasing concentration, while remaining nonzero, the same statement is true for the energy gap Ω_0. At a low impurity concentration ($a_i \ll 1$) we have

$$\begin{aligned} \Omega_0 &\simeq \Gamma_2 + \frac{\hbar}{2\tau_{21}}\sqrt{\frac{\xi - 1}{\xi + 1}} \quad \text{for } \Gamma_1 > \Gamma_2, \\ \Omega_0 &\simeq \Gamma_1 + \frac{\hbar}{2\tau_{12}}\sqrt{\frac{1 - \xi}{1 + \xi}} \quad \text{for } \Gamma_2 > \Gamma_1, \end{aligned} \tag{14}$$

where $\xi = \Gamma_1/\Gamma_2$.

For what follows, it is of interest to calculate the densities of states $\mathcal{N}_n$ in the neighborhood of $\Omega \simeq \Omega_0$. The calculations performed lead to the following results.

For $a_i \gg 1$,

$$\frac{\mathcal{N}_n(\Omega)}{N_n} \simeq \sqrt{\frac{2}{3}}\left(\frac{\Gamma_1\Gamma_2}{\Gamma_1 - \Gamma_2}\right)^{4/3}\frac{(a_1 + a_2)^2}{(a_1a_2)^{2/3}}\frac{\sqrt{\Omega - \Omega_0}}{\Omega_0^{11/6}}, \tag{15}$$

where by Ω_0 in the present case one should mean expression (13).

For $a_i \ll 1$ and $\Gamma_1 > \Gamma_2$:

$$\frac{\mathcal{N}_1(\Omega)}{N_1} \simeq \sqrt{\frac{2}{3}}\,\frac{\sqrt{\Omega-\Omega_0}}{\sqrt{\Gamma_2}}\,\frac{a_1^{1/3}}{a_2^{2/3}}\left(1+\frac{1}{\xi}\right)^{-1/2}\left(1-\frac{1}{\xi}\right)^{-5/6},$$
$$\frac{\mathcal{N}_2(\Omega)}{N_2} \simeq \sqrt{\frac{2}{3}}\,\frac{\sqrt{\Omega-\Omega_0}}{\sqrt{\Gamma_2}}\,(a_1a_2)^{-2/3}\left(1+\frac{1}{\xi}\right)\left(1-\frac{1}{\xi}\right)^{-1/3}, \tag{16}$$

and for $\Gamma_2 > \Gamma_1$:

$$\frac{\mathcal{N}_1(\Omega)}{N_1} \simeq \sqrt{\frac{2}{3}}\,\frac{\sqrt{\Omega-\Omega_0}}{\sqrt{\Gamma_1}}\,(a_1a_2)^{-2/3}(1+\xi)(1-\xi)^{-1/3},$$
$$\frac{\mathcal{N}_2(\Omega)}{N_2} \simeq \sqrt{\frac{2}{3}}\,\frac{\sqrt{\Omega-\Omega_0}}{\sqrt{\Gamma_1}}\,a_2^{1/3}a_1^{-2/3}(1+\xi)^{-1/2}(1-\xi)^{-5/6}. \tag{17}$$

On the basis of these results, for the low-temperature electronic heat capacity in the limit $a_i \gg 1$ we obtain:

$$C_s \simeq 2\sqrt{\frac{2\pi k_B}{3T}}\,(N_1+N_2)\Omega_0^{1/6}e^{-3\Omega_0}\left(\frac{\Gamma_1\Gamma_2}{\Gamma_1-\Gamma_2}\right)^{4/3}\frac{(a_1+a_2)^2}{(a_1a_2)^{2/3}}, \tag{18}$$

and in the case of a low impurity concentration $a_i \ll 1$,

$$C_s \simeq 2\sqrt{\frac{2\pi k_B}{3T}}\,\frac{\Omega_0^2 e^{+\beta\Omega_0}}{(a_1a_2)^{2/3}}\begin{cases}\dfrac{N_2}{\sqrt{\Gamma_2}}\,\dfrac{(1+1/\xi)}{(1-1/\xi)^{1/3}}, & \Gamma_1 > \Gamma_2,\\[2ex] \dfrac{N_1}{\sqrt{\Gamma_1}}\,\dfrac{(1+\xi)}{(1-\xi)^{1/3}}, & \Gamma_2 > \Gamma_1.\end{cases} \tag{19}$$

Let us now turn to the limiting case of temperatures close to the critical temperature T_c. In this case the parameters Γ_n are small. Expanding with respect to them,

$$\Gamma_n = \left(\ln\frac{\beta}{\beta_c}\right)^{1/2}\left[C_n + \ln\frac{\beta}{\beta_c}\,C_n^1 + ...\right], \tag{20}$$

we obtain, in the limit of a high impurity concentration ($\hbar\beta_c/2\tau_{nm} \gg 1$), the expressions

$$\frac{C_2}{C_1} = \frac{1-V_{11}N_1\ln(2\gamma\beta_c\omega_1/\pi)}{V_{21}N_2\ln(2\gamma\beta_c\omega_2/\pi)}, \qquad C^2 = \frac{8}{7\zeta(3)}\left(\frac{\pi}{\beta_c}\right)^2, \tag{21}$$

where

$$C = (C_1 N_1 + C_2 N_2)/(N_1 + N_2). \tag{22}$$

On the basis of these formulas and the expression for the difference of the thermodynamic potentials, obtained under the same assumptions, we obtain for the critical magnetic field H_c and the jump of the heat capacity C_s at the critical point the expressions

$$\frac{H_c^2}{8\pi} = \Lambda \left(\ln \frac{\beta}{\beta_c} \right)^2, \qquad C_s(T_c) - C_n(T_c) = 2\beta_c \Lambda, \qquad \Lambda = \frac{4}{7\zeta(3)} \left(\frac{\pi}{\beta_c} \right)^2 (N_1 + N_2). \tag{23}$$

The expressions obtained coincide in form with the analogous formulas for pure one-band substances if β_c is understood as the quantity determined on the two-band basis [(3)], and if it is assumed that, instead of the density of states of the one-band model, the total density $N_1 + N_2$ enters. Equation (23) also coincides in form with the analogous formulas for pure two-band substances in which interband transitions are absent, provided, however, that the quantity β_c is defined according to Ref. [(3)].

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Note: Figure translations are in progress. See original paper for figures.