

On Occasional Zeros of the Gap in Superconductors

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It has been shown that peculiar phase transitions of appearing occasional zeros of the gap of the electron spectrum can occur in superconductors at finite temperatures. The form of the thermodynamic features upon such disappearance of the gap on lines or at points of the Fermi surface has been determined.

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Volovik and Gor'kov [1] showed that isolated lines and (or) points at which the gap in the electron spectrum disappears exist in superconductors with a non-trivial violation of gauge invariance. Lines of zero gap in nonmagnetic superconductors and points in magnetic superconductors can also appear without any special cause. A transition of a superconductor from a state with a finite gap to a state with such occasional disappearance of the gap is similar to the Lifshits transition [2] changing the topology of the Fermi surface in metals. In contrast to transitions in metals, such topological transitions in superconductors are characterized by singular behavior at the temperature of the appearing zeros.

The order parameter in a usual superconductor is a complex function $\Delta e^{i\varphi}$, where the phase φ corresponds to the violation of gauge invariance and Δ is a real function of the quasimomentum orientation and determines the energy of the electronic excitation near the Fermi surface:

$$\varepsilon = \sqrt{\Delta^2 + v_F^2(q - q_F)^2}.$$

The function Δ is usually sign definite; in this case, $\Delta > 0$ can be taken in view of gauge invariance.

Near the minimum of the function Δ ,

$$\Delta \approx \Delta_0 + g(n_x^2 + n_y^2),$$

where the components n_x and n_y specify a small deviation of the quasimomentum orientation from the minimum direction. For the sake of simplicity, this orientation in the crystal is assumed to have symmetry higher than the second order.

The function Δ depends on the temperature and pressure. In particular, on a certain line $T_0(P)$, the minimum function value Δ_0 can vanish and change sign. Near such a critical line,

$$\Delta_0 = A(T - T_0).$$

Let us suggest that $A > 0$. In this case, at $T < T_0$, a zero gap line in the form of a small ring around the direction under consideration appears on the Fermi surface.

For low temperatures, the contribution from electronic excitations to the thermodynamic potential of the superconductor is given by the expression

$$\Omega = -T \int \ln(1 + e^{-\varepsilon/T}) \frac{d^3\mathbf{k}}{(2\pi)^3}. \quad (1)$$

Near the critical temperature T_0 in the potential given by Eq. (1), a singular part $\delta\Omega$ can be separated, which is a nonanalytic function of the small parameter

$$\tau = A \frac{T - T_0}{T_0}.$$

In terms of the appropriate dimensionless variables, the function $\delta\Omega$ is reduced to the integral

$$-\int_{-\infty}^{\infty} \ln\left(1 + e^{-\sqrt{(\tau + x^2 + y^2)^2 + z^2}}\right) dx dy dz.$$

Let us pass to the variable $\eta = \tau + x^2 + y^2$ and $\theta(\tan\theta = y/x)$. The integration with respect to the angle θ yields

$$\delta\Omega \propto -\int_{\tau}^{\infty} d\eta \int_{-\infty}^{\infty} dz \ln(1 + e^{-\sqrt{\eta^2 + z^2}}).$$

From this expression, a singular (obtained when differentiating with respect to τ) contribution to the heat capacity is expressed as

$$\delta C \propto -\int_{-\infty}^{\infty} \frac{1}{e^{\sqrt{\tau^2 + z^2}} + 1} \frac{\tau dz}{\sqrt{\tau^2 + z^2}}.$$

The integration with logarithmic accuracy provides

$$\delta C \propto -\tau \ln \frac{1}{|\tau|}.$$

Thus, the heat capacity must increase sharply with a decreasing temperature near T_0 .

In superconductors with broken time reversal symmetry, the order parameter

$$(\Delta_1 + i\Delta_2)e^{i\varphi}$$

is determined by two linearly independent functions Δ_1 and Δ_2 of the quasimomentum orientation [3]. These functions are transformed according to certain one-dimensional representations or to a certain two-dimensional representation of the crystallographic symmetry group of the crystal. For a particular representation, the symmetry-induced zero lines must exist for each of these functions. At the points of the intersection of zero lines of different functions, there are energy gap zero points:

$$\Delta = \sqrt{\Delta_1^2 + \Delta_2^2}.$$

Occasional zero gap points appear when a occasional zero line appears for one of the functions, e.g., Δ_2 (as was considered for a nonmagnetic case) and intersects the existing zero line of the function Δ_1 .

Let us consider a case where the ring of vanishing the function Δ_2 appears immediately over the zero line of the function Δ_1 , which is attributed to symmetry. Near this direction,

$$\Delta_1 \propto n_y,$$

$$\Delta_2 = \Delta_0 + g_{xx}n_x^2 + g_{yy}n_y^2.$$

It is easy to verify that the n_y dependence of the function Δ_2 can be disregarded when determining thermodynamic features. In this case, in terms of the appropriate dimensionless variables, the contribution of the electronic excitations to the thermodynamic potential given by Eq. (1) is reduced to the integral

$$\Omega \propto - \int_{-\infty}^{\infty} \ln \left(1 + e^{-\sqrt{(\tau+x^2)^2 + y^2 + z^2}} \right) dx dy dz.$$

Let us pass to the variable $\eta = y^2 + z^2$ and θ ($\tan \theta = z/y$). The integration with respect to the angle θ yields

$$\delta \Omega \propto - \int_0^{\infty} d\eta \int_{-\infty}^{\infty} dx \ln \left(1 + e^{-\sqrt{(\tau+x^2)^2 + \eta}} \right).$$

From this expression, a singular contribution to the entropy is expressed as

$$S \propto - \int_0^{\infty} \int_{-\infty}^{\infty} \frac{d\eta dx}{e^{\sqrt{(\tau+x^2)^2 + \eta}} + 1} \frac{\tau + x^2}{\sqrt{(\tau+x^2)^2 + \eta}}.$$

Then, the integration with respect to the variable η can be performed:

$$S \propto - \int_{-\infty}^{\infty} dx (\tau + x^2) \ln(1 + e^{-|\tau+x^2|}).$$

For $\tau > 0$, the entropy is given by the expression

$$S_r \propto - \int_{-\infty}^{\infty} dx (\tau + x^2) \ln(1 + e^{-\tau-x^2}). \quad (2)$$

For $\tau < 0$, the entropy can be represented in the form of the sum of two terms. The first term is the regular contribution given by Eq. (2) and the second term is the singular contribution

$$\delta S \propto - \int_0^{\sqrt{-\tau}} dx (\tau + x^2) \ln \frac{1 + e^{\tau+x^2}}{1 + e^{-\tau-x^2}}.$$

Here, the integrand can be expanded in terms of small τ and x quantities and integration can be performed. Finally, the singular heat capacity is obtained in the form

$$\begin{aligned} \delta C &\propto (-\tau)^{3/2}, \quad \tau < 0, \\ \delta C &= 0, \quad \tau > 0. \end{aligned}$$

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