Singularities of the energy "gap" of a superconductor

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The existence of singularities in the energy "gap" $\Delta(\mathbf{p},\omega)$ in $(\mathbf{p},\omega)$ space is predicted. It is shown that in the general case the singularities in $\Delta(\mathbf{p},\omega)$ are due to a change in the topology of the line of intersection of the Fermi surface with the phonon equal-energy surfaces.

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It is known that the energy "gap" $\Delta(\mathbf{p},\omega)$ as a function of the momentum **p** and the frequency ω is a generalized order parameter of a superconductor and is determined by solving the Éliashberg equations.[1] In experiment, the average value of the "gap" $\Delta(\omega)=\langle\Delta(\mathbf{p},\omega)\rangle_{\mathbf{p}}$ is usually determined from the tunnel characteristics of polycrystals.[2] It is known that $\Delta(\omega)$ has singularities as a function of the parameter ω.[2] It was proposed[3] that the singularities of $\Delta(\omega)$ can be due only to an irregular addition to the density of the number of states of the phonons when the topology of the phonon equal-energy surfaces is altered. The different equal-energy surfaces of the phonons manifest themselves in the external paramter ω. Naturally, the singularities of $\Delta(\omega)$ are a consequence of the singularities of $\Delta(\mathbf{p},\omega)$. The nature of the possible singularities of $\Delta(\mathbf{p},\omega)$ in $(\mathbf{p},\omega)$ space is investigated in this paper from a unified point of view.

It is known that the quantity $\Delta(\mathbf{p},\omega)=\phi(\mathbf{p},\omega)/Z(\mathbf{p},\omega)$ is obtained by solving the system of equations for the function $\phi(\mathbf{p},\omega)$ and the parameter $Z(\mathbf{p},\omega)$.[1,3,4] The real and imaginary parts of the functions $\phi(\mathbf{p},\omega)$ and $Z(\mathbf{p},\omega)$ satisfy the Cauchy relation.[1,3,4] Therefore to determine the singularities in $\Delta(\mathbf{p},\omega)$ it suffices to determine them for the imaginary parts of $\phi(\mathbf{p},\omega)$ and $Z(\mathbf{p},\omega)$. Since the structure of the singularities in $\phi(\mathbf{p},\omega)$ and $Z(\mathbf{p},\omega)$ is the same, we confine ourselves to a study of the singularities in $\phi(\mathbf{p},\omega)$.

Let for the sake of argument $\omega>0$. Then, following[1,3,4], we represent the function $\mathrm{Im}\phi(\mathbf{p},\omega)$ in the form

$$\mathrm{Im}\,\phi(\mathbf{p},\omega) = -\int_0^{\omega} d\omega'\,\mathrm{th}\frac{\omega'}{2T}\int\frac{d\mathbf{p}'}{(2\pi)^3}\,\mathrm{Im}\left\{\frac{\phi(\mathbf{p}',\omega')}{Q(\mathbf{p}',\omega')}\right\}\sum_{\lambda}|g^{\lambda}_{\mathbf{p},\mathbf{p}'}|^2\,\delta(\omega_{\lambda}(\mathbf{p}-\mathbf{p}') + \omega' - \omega),$$

$$Q(\mathbf{p},\omega) = \omega^2 Z^2(\mathbf{p},\omega) - \phi^2(\mathbf{p},\omega) - \xi^2(\mathbf{p});\ \xi(\mathbf{p}) = \epsilon(\mathbf{p}) - \mu. \tag{1}$$

Here $\epsilon(\mathbf{p})$ is the renormalized electron energy, g is the electron-phonon interaction parameter, μ is the chemical potential, T is the temperature, and λ is the number of the branch of the phonon spectrum. To investigate the singularities in $\phi(\mathbf{p},\omega)$, it is convenient to change over from integration with respect to dp' to integration with respect to the variables $\epsilon(\mathbf{p}')$, $\omega_\lambda(\mathbf{p}-\mathbf{p}')$, and the length $l^{\lambda}_{\mathbf{p}'}$ of the contour of the line at which the surfaces $\epsilon(\mathbf{p}')=\epsilon$ and $\omega_\lambda(\mathbf{p}-\mathbf{p}')=\omega$ intersect (hereafter the "$l^{\lambda}_{\mathbf{p}'}$ line" for brevity), and forego the transition to the variables $\epsilon(\mathbf{p}')$ and an arbitrary orthogonal coordinate system on the $\epsilon(\mathbf{p}')=\epsilon$ surface, which is customarily employed in superconductivity theory.[1,3,4] In the general case, there may be several such $l^{\lambda}_{\mathbf{p}'}$ lines, owing to the multiple-valuedness and periodicity of the functions $\epsilon(\mathbf{p}')$ and $\omega_\lambda(\mathbf{p}-\mathbf{p}')$. We note that the length of the $l^{\lambda}_{\mathbf{p}'}$ line depends on the external parameters $\mathbf{p}$ and ω. Carrying out the integration in (1), we obtain an expression for $\mathrm{Im}\phi(\mathbf{p},\omega)$ in the form

$$\mathrm{Im}\,\phi(\mathbf{p},\omega) = \pi\int_0^{\omega} d\omega'\,\mathrm{th}\frac{\omega'}{2T}\sum_{\lambda}\int\frac{dl^{\lambda}_{\mathbf{p}'}\,|g^{\lambda}_{\mathbf{p}\mathbf{p}'}|^2}{|S^{\lambda}_{\mathbf{p}-\mathbf{p}'}(\omega-\omega')|\,|v_{\mathbf{p}'}(\mu)|\sin\theta_{\mathbf{p}'}}$$

$$\times\,\mathrm{Re}\left\{\frac{\Delta(\mathbf{p}',\omega')}{\sqrt{\omega^2-\Delta^2(\mathbf{p}',\omega')}}\right\} \tag{2}$$

Here $\theta_{\mathbf{p}'}$ is the angle between the vectors $\mathbf{v}_{\mathbf{p}'}(\epsilon)=\nabla_{\mathbf{p}'}\epsilon(\mathbf{p}')\,|_{\epsilon(\mathbf{p})=\epsilon}$ and $\mathbf{S}^{\lambda}_{\mathbf{q}}(\omega)=\nabla_{\mathbf{q}}\omega_\lambda(\mathbf{q})\,|_{\omega_\lambda(\mathbf{q})=\omega}$, and depends on $\mathbf{p}$ and ω.

It follows from (2) that if the external parameters p and ω are varied, then $\phi(\mathbf{p},\omega)$ can have at $\mathbf{p}=\mathbf{p}^*$ and $\omega=\omega^*$ the following singularities: (1) at the points $\mathbf{p}'=\mathbf{p}'_0$, at which $\sin\theta_{\mathbf{p}'_0}=0$, (2) at the points $\mathbf{p}'=\mathbf{p}^*-\mathbf{q}_k$, at which $S^{\lambda}_{\mathbf{q}_k}(\omega^*)=0$. The geometrical interpretation of these cases is the following. In the first case the surfaces $\epsilon(\mathbf{p}'_0)=\mu$ and $\omega_\lambda(\mathbf{p}^*-\mathbf{p}'_0)=\omega^*$ are tangent at the point $\mathbf{p}'_0$. This is the analog of the Kohn singularity.[5-7] The peculiarity of the Kohn singularities lies in this case in the fact that, besides satisfaction of the usual condition $q=2p^*_{\mathrm{extr}}$ it is necessary that the vectors $\mathbf{v}_{\mathbf{p}^*}(\mu)$ and $\mathbf{S}^{\lambda}_{\mathbf{q}}(\omega)$ be parallel or antiparallel ($2p^*_{\mathrm{extr}}$ is the extremal diameter of the Fermi surface). These conditions are satisfied, for example, in the case $q_{\mathrm{extr}}=2p^*_{\mathrm{extr}}$ ($2q_{\mathrm{extr}}$ is the extremal diameter of the surface $\omega_\lambda(\mathbf{q})=\omega^*$). In the second case, the surface $\epsilon(\mathbf{p}')=\mu$ crosses the surface $\omega_\lambda(\mathbf{q})=\omega^*$ near directions of $\mathbf{q}_k$, where the topology of the phonon equal-energy surfaces changes. The topological singularities of the phonon spectrum manifest themselves if the surfaces $\epsilon(\mathbf{p}^*)=\mu$ and $\epsilon(\mathbf{p}^*-\mathbf{q}_k)=\mu$ have either an intersection line or a tangency line.

In the cases considered, the $l^{\lambda}_{\mathbf{p}'}$ line changes its topology in an infinitesimally small vicinity of the points $\mathbf{p}'=\mathbf{p}_0'$ and $\mathbf{p}'=\mathbf{p}^*-\mathbf{q}_k$. The most characteristic topological changes are those in which the $l^{\lambda}_{\mathbf{p}'}$ either degenerates to a point (elliptic point) or has a self-intersection point (hyperbolic point).

We note that the singularities of the integral with respect to $dl^{\lambda}_{\mathbf{p}'}$ are similar to the singularities of the absorption coefficient of ultrasound in metals.[7,8]

The calculations show that at $\mathbf{p}=\mathbf{p}^*$ and $\omega=\omega^*$ the integral with respect to $dl^{\lambda}_{\mathbf{p}'}$ has a singular part for which the analytic expressions depends essentially on the character of the topological singularities of the $l^{\lambda}_{\mathbf{p}'}$ line. We note that integration with respect to ω does not lower the singularities of the integral with respect to $dl^{\lambda}_{\mathbf{p}'}$, because of the root singularity of the integrand $[\omega^2-\Delta^2(\mathbf{p},\omega)]^{1/2}$, which is proportional to the density of the number of states of the quasiparticles in the superconductor.

To establish the form of the singularity in $\mathrm{Im}\phi(\mathbf{p},\omega)$, we calculate its derivative $\partial\,\mathrm{Im}\phi(\mathbf{p},\omega)/\partial\omega$ at $T=0$:

$$\frac{\partial\,\mathrm{Im}\,\phi(\mathbf{p}^*,\omega)}{\partial\omega}\sim\begin{cases}\pm[(\omega-\omega^*)^2-\Delta^{*2}]^{-1/2}\,\theta[(\omega^*+\Delta^*)-\omega]\\[2ex] -[\Delta^{*2}-(\omega-\omega^*)^2]^{-1/2}\,\theta[\omega-(\omega^*+\Delta^*)]\end{cases},\qquad(3)$$

where $\Delta^*=\Delta[\mathbf{p}',\Delta(\mathbf{p}')]$ is obtained by solving the equation $\omega^2-\Delta^2(\mathbf{p}',\omega)=0$, and the momentum $\mathbf{p}'$ takes on a value either $\mathbf{p}_0'$ or $\mathbf{p}^*-\mathbf{q}_k$. For the sake of clarity we have presented the calculation results for two cases of topological singularities of the $l^{\lambda}_{\mathbf{p}'}$ line–the upper line of (3)–elliptic point ("+" corresponds to appearance of the $l^{\lambda}_{\mathbf{p}'}$ line with increasing ω, and "−" to its vanishing), and the lower line corresponds to the hyperbolic point. It follows from (3) that $\partial\,\mathrm{Im}\phi(\mathbf{p},\omega)/\partial\omega$ has a root singularity at $\omega=\omega^*+\Delta^*$. Using the Cauchy relation, we can show that the singular part of $\partial\,\mathrm{Re}\phi(\mathbf{p},\omega)/\partial\omega$ also has a root singularity.

Thus, according to the foregoing analysis, in the general case the quantity $\Delta(\mathbf{p},\omega)$ can have in $(\mathbf{p},\omega)$ space singularities connected with the change of the topology of the line of intersection of the Fermi surface with the phonon equal-energy surfaces. These singularities[3] in $\Delta(\mathbf{p},\omega)$ lead to a larger class of singularities in $\Delta(\omega)$ than hitherto assumed. We note that the singularities of $\Delta(\omega)$, which are due to the change of the topology of the $l^{\lambda}_{\mathbf{p}}$ line near q_k, are of the same form as in[3] only when the surfaces $\epsilon(\mathbf{p})=\mu$ and $\epsilon(\mathbf{p}-\mathbf{q}_k)=\mu$ have an intersection line.

If we consider as an external parameter, besides $\mathbf{p}$ and ω, also the pressure P, then in phase transitions of order $2\frac{1}{2}$ [9] the quantity $\Delta(\mathbf{p},\omega)$ acquires in $(\mathbf{p},\omega)$ space singularities due to the change of the topology of the $l^{\lambda}_{\mathbf{p}'}$ line near the directions $\mathbf{p}'=\mathbf{p}_k$, where the topology of the Fermi surface changes. These singularities will be observed at $P\approx P^*$ for all values of $\mathbf{p}$ and ω satisfying the conditions $\omega_\lambda(\mathbf{p}-\mathbf{p}_k)=\omega$ and $\epsilon(\mathbf{p})=\mu$. The value P^* corresponds to the pressure when $|\mu-\epsilon_k|\sim mS^2/2$, where m is the electron mass, S is the speed of sound, and $\epsilon_k=\epsilon(\mathbf{p}_k)$ is the critical energy.

The considered singularities in the energy "gap" $\Delta(\mathbf{p},\omega)$ can apparently be observed in experiments on tunnel effects in single-crystal superconductors. Observation of these singularities would uncover new possibilities in the investigation of the singularities of both the phonon and the electron spectra of superconductors.

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