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Temperature effect on the quasiparticle spectrum of an impurity-doped superconductor with two separate electron groups

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The two-gap BCS theory with incoherent single-particle scattering is applied to study the temperature dependence of the quasiparticle density of states in a superconductor with two separate electron groups. It is shown that in such a material nonmagnetic impurities can affect superconductivity in a nontrivial way. For considerable intergroup scattering rates comparable with clean-limit gap magnitudes we find a crossover from two-feature densities of states at low temperatures to standard BCS-type curves with a single maximum, as T increases. We point out that some unexpected temperature-dependent features observed for magnesium diboride, a two-band superconductor, may not represent its intrinsic characteristics.

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The well-known Anderson theorem[1] relating elastic scattering centers in a bulk superconductor that do not affect its pair potential is applied only to initially isotropic and homogeneous systems. A specific case of a system without translational symmetry is a normal-metal (N)–superconductor (S) sandwich where, as it was shown by Arnold,[2] the Anderson theorem is not satisfied. Its inapplicability results, first of all, in the homogenization of pair potentials over the N and S layers. In fact, this conclusion is valid not only for proximity-effect bilayers but also for a variety of inhomogeneous superconducting structures. It is remarkable that the results of Ref. 2 for very thin N and S layers bear a striking resemblance to the McMillan tunneling model[3] of the proximity effect proposed for two N and S layers separated by a tunnel barrier. The correspondence arises from a similar treatment of lifetime effects. It is also not surprising that analogous expressions are appropriate for multiband superconductors with nonmagnetic impurity scattering treated within the Born approximation.[4,5] As in the general case of an anisotropic superconductor,[6] interband scattering reduces the critical temperature T_c and finally leads to a single order parameter.[5,7]

A specific but representative case of a multiband superconductor is a two-band–two-gap model originally proposed in 1959,[8,9] where the order parameter has two different magnitudes in two distinct bands. Recently, it became evident that the model may be directly applied to magnesium diboride, a superconducting material with an unexpectedly high critical temperature $T_c=39$ K.[10] Whereas the main physics behind superconductivity in clean samples of the compound is now well understood,[10] the role of incoherent single-particle scattering effects between the two bands in MgB_2 remains to a great extent unclear in doped[11] and clean samples. For example, the interband impurity scattering rates $\Gamma=1/(2\tau)$ (τ being the electron lifetime) deduced earlier from experiments on the T_c suppression using a weak-coupling BCS-type approach to the two-band case are underestimated.[12] Γ's for compact samples and thin films of MgB_2 found from point-contact and tunneling experiments ranged from 1 to 4 meV,[13,14] and were comparable with the lower gap magnitude of 2–3 meV. Even more surprising are recent results by Kohen *et al.*[15] who showed that also for single crystals of magnesium diboride an impact of elastic scattering between the bands should be taken into account in order to interpret in detail all tunneling spectroscopic features. The Γ values were found as great as 1–2 meV. It means that interband normal mixing is an important factor even in clean samples of magnesium diboride.

The best way to study experimentally disorder-induced changes in a superconductor with two separate electron groups is to measure its quasiparticle density of states $N(E)$, which contains information about gap functions in both groups and can be probed by various experimental techniques. The two densities of states $N_{1,2}(E)$ were calculated for very low temperatures in various papers (see, for example, Refs. 3–5, 16, and 17. The general feature of the weak-coupling limit is the presence of a single excitation gap E_g instead of two gaps $\Delta_{1,2}$ in the clean limit and prominent structures above the gap in partial self-energies, reflecting the real decay processes into another electron group. The strong-coupling formalism provides additional self-energy effects arising due to the electron-phonon interaction and a small filling of the gap due to thermal phonons.[17] The overall shapes of $N_{1,2}(E)$ radically depend on the ratio of the interband scattering rates Γ to the gap magnitude (see Fig. 4 in Ref. 17 varying from two BCS-like curves to a Cooper-like limit with almost the same densities of states for both groups (see Fig. 8 in Ref. 3). In this paper we want to attract attention to the fact that such gradual changes can be observed also for fixed Γ's as temperature is increased from zero to T_c. Below we study how the two very different densities of states $N_{1,2}(E)$ at $T=0$ become integrated with increasing temperature if the Γ's are comparable with the initial gap magnitudes. In other words, it means that the existence of two different gaps in a superconductor and incoherent scattering between the electron groups can produce a restoration of the

Anderson theorem with temperature and, as a result, a crossover from two-feature densities of states to conventional BCS characteristics with a single maximum. At the end of the paper we relate the nontrivial behavior of the $N_{1,2}(E)$ to an unexpected energy-gap temperature dependence for magnesium diboride observed by some experimental groups. In this work we remain within a weak-coupling approximation. Because magnesium diboride belongs to an intermediate-coupling regime,[18] our predictions concerning this compound should be regarded as qualitative ones. What we want to do is not to describe experimental curves for MgB_2 but rather to make some principal conclusions about sensitivity of temperature-dependent spectroscopic data for a superconductor with two electron groups to impurity scattering effects.

The normalized electronic densities of states $N_i(E)$ ($i=1, 2$) as functions of energy E are given by the expression

$$N_i(E) = N_i(0)\mathrm{Re}\frac{E}{\sqrt{E^2-\Delta_i^2(E)}}, \tag{1}$$

with $N_i(0)$, the partial normal-state densities of states at the Fermi levels, and $\Delta_i(E)$ the related temperature-dependent complex gap functions. The total tunneling characteristic $N(E)$ for a certain direction includes both terms with weights that are determined by the topology of the Fermi surfaces and corresponding Fermi velocities. The order parameters $\Delta_i(E)$ should be found self-consistently from two equations including the two-band extension of the standard BCS theory[8,9] and finite lifetime effects[3]

$$\Delta_i(E) = \frac{\sum_{j=1,2}\left\{\Lambda_{ij}\int_0^{\omega_0} d\varepsilon\,\tanh(\varepsilon/2k_\mathrm{B}T)\mathrm{Re}[\Delta_j(\varepsilon)/\sqrt{\varepsilon^2-\Delta_j^2(\varepsilon)}] + i[\Gamma_{ij}\Delta_j(E)/\sqrt{E^2-\Delta_j^2(E)}]\right\}}{1+\sum_{j=1,2}[\Gamma_{ij}/\sqrt{E^2-\Delta_j^2(E)}]}; \tag{2}$$

here $\Lambda_{ij}=N_j(0)V_{ij}$ are dimensionless coupling constants, V_{ij} are the partial pairing potentials, ω_0 is the cutoff energy, and Γ_{ij} describe the scattering rates inside and between the groups. It directly follows from Eq. (2) that intragroup scattering terms with Γ_{ii} compensate each other and the only remaining contribution is that from off-diagonal scattering effects. Within the Born approximation $\Gamma_{ij}=1/(2\tau_{ij}) = \pi n_\mathrm{imp}N_j(0)\langle|W_{ij}|^2\rangle/2=\mathrm{const}$, where n_imp is the nonmagnetic impurity concentration, $\langle|W_{ij}|^2\rangle$ are the averaged-over-angles matrix elements determined by incoherent scattering between states in the two electron groups, the ratios $\Gamma_{ij}/\Gamma_{ji} =\Lambda_{ij}/\Lambda_{ji}=N_j(0)/N_i(0)$.

To imitate the properties of magnesium diboride, a two-band–two-gap superconductor, we chose the following parameters: $\Lambda_{11}=0.3$, $\Lambda_{12}=0.15$, $\Lambda_{21}=\Lambda_{22}=0.1$, $\omega_0=50$ meV. Then in the clean limit ($\Gamma_{12}=\Gamma_{21}=0$) we get two gap values $\Delta_1=7.2$ meV, $\Delta_2=2.8$ meV (here and below we assume that the energy-gap magnitude in the clean limit is lower for the second electron group) and the critical temperature slightly above 40 K which qualitatively corresponds to related parameters for MgB_2.[10] Our aim is to perform calculations for a dirty system of two coupled electron groups. It should be noticed that in this case the Born approximation is not valid near the energy gap that has now a single value E_g defined by an equality $E_g=\mathrm{Re}\,\Delta_2(E_g)$. Because of it, in this region we have to treat the impurity-induced term in the Hamiltonian to all orders of self-consistent perturbation theory as was done before by Mohabir and Nagi[16] for the McMillan tunneling model of the proximity effect. Then the lifetime broadening characteristics in Eq. (2) become energy-dependent complex quantities $\tilde{\Gamma}_{ij}=1/[2D(E)\tau_{ij}]$ with

$$D(E) = 1 + 2c\frac{E^2-\Delta_1(E)\Delta_2(E)}{\sqrt{E^2-\Delta_1^2(E)}\sqrt{E^2-\Delta_2^2(E)}} \tag{3}$$

and the parameter c controlling the renormalization effect,[16] $c=(4\tau_{12}\tau_{21}/\langle|W_{12}|^2\rangle)^{-1}$. For the Γ's used in our calculations we have estimated the value of c to be less than or nearly 0.01. Its renormalization effect [the cancellation of the singularities in Eq. (2) at $E=E_g$] is important only in the vicinity of the gap value.

As follows from Eq. (2), imaginary parts of the order parameters are vanishing for very high energies and $\Delta_i(E)$ are going asymptotically to temperature-dependent constants Δ_i^0 which for small T are nearly the clean-limit gap magnitudes at $T=0$ but strongly differ from them for greater temperatures. For energies lower than Γ, the functions $\Delta_i(E)$ are close to each other. In the gap region the densities of states $N_{1.2}(E)$ defined by Eq. (1) exhibit two main features at energies that are nearly solutions of the equation

$$E = \mathrm{Re}\,\Delta_{1,2}(E). \tag{4}$$

In the clean limit the relations (4) set positions of distinct peaks in the densities of states $N_{1.2}(E)$ (crossings of dashed lines with a dotted one in Fig. 1). For Γ's comparable with ω_0 the densities of states and gap values for both electron groups are almost the same.[7] Less trivial is the intermediate case when the intergroup scattering rates are comparable with clean-limit gap magnitudes. For Γ's not too great we again obtain two different solutions of Eq. (4) (intersections of curves 1 and 1′ with a dotted line in Fig. 1). But if the scattering rates essentially exceed Δ_i^0 the distance between them becomes very short and we can observe a crossover to

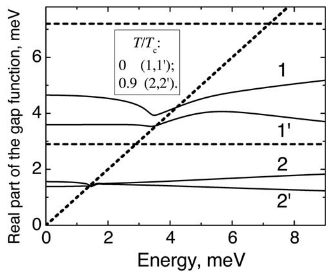

FIG. 1. Real parts of energy gap functions $\mathrm{Re}\,\Delta(E)=E$ for zero temperature (curves 1 and $1'$) and $T=0.9T_c$ (curves 2 and $2'$) of a superconductor with two electron groups. Here and below the parameters are chosen as follows: $\Lambda_{11}=0.3$; $\Lambda_{12}=0.15$; $\Lambda_{21}=\Lambda_{22}=0.1$; $\Gamma_{12}=6.0$ meV; $\Gamma_{21}=4.0$ meV; $c=0.01$; $\omega_0=50$ meV. The critical temperature T_c is estimated to be nearly 33 K. Curves 1, 2 and $1'$, $2'$ are the data for larger-gap and smaller-gap groups, respectively; the dotted straight line is $\mathrm{Re}\,\Delta(E)=E$. The dashed lines are the predictions for the clean limit when $\Gamma_{12}=\Gamma_{21}=0$.

a situation similar to an ordinary single-band superconductor (see also Figs. 3 and 4 in Ref. 5).

In a real experiment it is impossible to control gradual modifications of the Γ's. But the crossover discussed can be realized with temperature as a parameter that changes the relation between initial Δ_i^0 and the scattering rates. If the Γ's are not too high, for low T's we get curves $N_{1,2}(E)$ with two distinct features. Increasing the temperature, we suppress the gap values but do not change essentially the Γ's, which for conventional superconductors have little temperature dependence below T_c. In this way, we realize a situation when both solutions of Eq. (4) (intersections of curves 2 and $2'$ with a dotted line in Fig. 1) almost coincide. The disappearance of the gap anisotropy means a restoration of the Anderson theorem with two nearly identical densities of states exhibiting strong singularities at the gap value E_g. Dramatic modifications of the normalized densities of states $N_i(E)/N_i(0)$ can be seen in Fig. 2. It is evident that the effect discussed should take place in all dirty superconducting samples with two separate electron groups. The temperature range where it could be observed depends on the ratio of Γ_{ij} to Δ_i^0. For comparatively small Γ's it is limited by the nearest vicinity of T_c as in Ref. 17 where the evolution of the superconducting densities of states for MgB_2 was calculated within the framework of the two-band Eliashberg theory. As follows from Fig. 2, the density of states $N_1(E)$ of the larger-gap group can survive drastic changes in the intermediate range of temperatures: the increase of T strongly suppresses a maximum recalling the gap in the first electron group and gives rise to a peak at $\sim E_g$. Note that the authors of Ref. 17 have also mentioned the fact that the temperature-induced non-BCS changes in the densities of states of doped MgB_2 are more pronounced for a sample with a larger gap.

Let us now turn to an unexpected energy-gap temperature dependence for magnesium diboride derived by some experimental groups from tunneling and point-contact experiments. For sufficiently clean samples, where two clear gaps were revealed, their behavior with increasing T is qualitatively similar to that predicted by the classic BCS theory, except of the lower-gap data suppression near T_c.[14,19] According to Nicol and Carbotte[20] such behavior could be explained within the two-band scenario in the limit of nearly separate bands with small interband scattering rates. Much more dramatic suppression in the intermediate temperature range was found for MgB_2 samples that could be supposed as dirty ones. Comparison of early experimental data with strong-coupling calculations of the energy-gap temperature dependence reveals this tendency for a larger gap (see Fig. 3 in Ref. 21). Even more striking results were observed in samples exhibiting a single energy gap that considerably deviated from the corresponding rescaled BCS curve in a wide region between $T=0$ and $T=T_c$.[22,23] It contradicts an intuitive feeling that an isotropic, dirty-limit gap should follow the BCS behavior.[23] We attribute the observations to dramatic changes in the $N_1(E)$ seen in our Fig. 2 that can occur for Γ's comparable with clean-limit gap magnitudes. In experiments gap values are usually found from the positions of the two maxima in the total density of states [or other features that appear in the experimental characteristics, in fact, due to the presence of the peaks in $N_i(E)$]. It is clear from Figs. 1 and 2 that for a dirty superconductor the position of the higher-energy maximum at $T=0$ has no clear physical meaning. Moreover, the feature gradually shifts to lower energies with increasing temperature, merging with a lower-energy peak

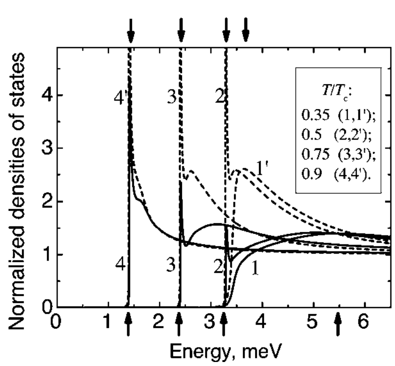

FIG. 2. The temperature effect on the normalized densities of states $N_i(E)/N_i(0)$. Curves 1–4 and $1'$–$4'$ are the data for larger-gap and smaller-gap groups, respectively. Arrows below and above the figure show the main peak positions in the $N_1(E)$ and $N_2(E)$ characteristics. The calculations have been done for the parameters indicated in the caption to Fig. 1.

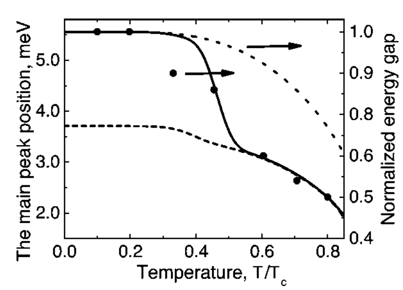

FIG. 3. The temperature behavior of the main peak positions in the two densities of states, shown with arrows above and below Fig. 2 (the left axis), compared with experimental data (Ref. 22) for normalized energy-gap values shown by circles. The dotted curve represents the BCS behavior. The calculations have been done for the parameters indicated in the caption in Fig. 1.

near $T = T_c$. Figure 3 exhibits the nonmonotonic temperature-induced behavior of the main peak positions in the two densities of states shown with arrows above and below Fig. 2. It is compared with the anomalous temperature dependence of the normalized energy-gap value revealed in experiments with dirty samples of magnesium diboride.[22] Such findings can lead to an erroneous conclusion about the unconventional physical mechanism behind the effect whereas the unexpected temperature-dependent features in the density of states of a dirty two-group superconductor do not really represent intrinsic characteristics of the material. This conclusion is especially important for the electron transport measurements in magnesium diboride within the *ab* plane where the larger-gap band contribution is essential.[7]

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