Self-energy Effect of Superconducting Energy Gap in Point-Contact Spectra of MgB$_2$

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Introduction.

It is commonly accepted that the mechanism of superconductivity in recently discovered MgB$_2$ is due to the electron-phonon interaction (EPI). Among the known $s-p$ metals, the record breaking critical temperature ($T_c \approx 40 \text{ K}$) and the unusual two-band character in its electronic structure make this compound very interesting for detailed study. MgB$_2$ crystallizes in a hexagonal lattice with alternating planes of Mg and B. Up to now, there has been no detailed experimental determination of its EPI spectral function. The reason is that EPI in MgB$_2$ is strongly anisotropic, and single crystals, well suited for anisotropic measurements by means of tunneling or point-contact spectroscopy, are still under development. As for the tunneling spectroscopy, in order to extract the so-called "driving force" for high $T_c$ in this compound caused by EPI along the $ab$-plane, one needs a plane tunnel junction oriented perpendicular to this direction, which is not an easy task. On the other hand, the tunneling spectra in the $c$-direction are supposed to be so weak (see below), that the precise standard procedure for extracting the EPI function is difficult to apply. In Ref. it was shown that the inversion of the Eliashberg equation for a multiband superconductor is a mathematically ill-defined problem. The previous attempt to obtain a solution on polycrystalline samples contains an uncontrolled mixture of the two bands with a predominant contribution of the $\sigma$-band. The interaction of the two bands to a great extent determines the corresponding EPI functions. Their intensity depends on electron mean free path in each band separately. On the one hand, in some experiments the two bands can be considered as being independent of each other, but, on the other hand, both of them have the same $T_c$, despite quite different EPI. The layered structure and strongly anisotropic EPI allow us to hope that the peculiarities in MgB$_2$ may shed some light on the mechanism of high-$T_c$ superconductivity in copper oxides.

In the previous paper it was shown qualitatively that the phonon singularities in the point-contact spectra of the $c$-axis oriented MgB$_2$ thin films were due to the non-linear dependence of excess current $I_{exc}(eV)$ at energies higher than the superconducting energy gap $\Delta$. In the present contribution we derive asymptotic expressions for differential conductance of $N-c-S$ ($c$ stands for "constriction") point-contacts and show that quantitatively (within a factor of order of unity) the calculated point-contact spectra agree with the experimental data for the $c$-axis orientation of MgB$_2$, where only the $\sigma$-band is visible.

Theory.

The electronic structure of MgB$_2$ consists of two groups of bands: a pair of approximately isotropic 3D $\pi$-bands, and a pair of strongly anisotropic 2D $\sigma$-bands whose characteristics are measurable for the point contact oriented within a few degrees around the $ab$-plane. As it was argued in, the variation of the superconducting gap inside the $\sigma$- or the $\pi$-bands can hardly be observed in real samples due to intraband impurity scattering. Therefore, superconducting properties of MgB$_2$ can be described by an effective two-band model, where each group of the $\sigma$- and the $\pi$-bands is characterized by the corresponding order parameters $\Delta_{\sigma}$ and $\Delta_{\pi}$. The gap functions $\Delta_{\sigma,\pi}(E)$ in MgB$_2$ in the Matsubara representation, suitable for the description of thermodynamic properties, were calculated in Ref. from the solution of the Eliashberg equations using the theoretically calculated EPI spectral functions for the effective two-band model. Here we extend this approach to obtain the complex gap parameters $\Delta_{\sigma,\pi}(E)$ in MgB$_2$ as a functions of
Ref. [12] for the current-voltage dependence: the differential conductance follows from formula (21) from Ref. [11]:

\[
\left( \frac{dI}{dV} \right)_{\text{bal}} (eV) = \frac{1}{R_N} \left( 1 + \frac{\Delta(e)}{\epsilon + \sqrt{\epsilon^2 - \Delta^2(e)}} \right)^2 \epsilon = eV,
\]

where \( R_N \) is the normal state resistance.

In the dirty contact (\( l \ll d \)), the regime of current flow is diffusive and the corresponding expression for the differential conductance follows from formula (21) from Ref. [12] for the current-voltage dependence:

\[
I(V) = \frac{V}{R_N} + \frac{1}{eR_N} \int_0^{eV} \frac{d\epsilon}{2\sqrt{\epsilon^2 - \Delta^2(\epsilon)}} \times \left[ \frac{\text{Re} \frac{u}{\sqrt{u^2 - 1}} \left( \frac{\text{Re Arcsin} \left( \frac{1}{\sqrt{u^2 - 1}} \right)}{\text{Re} \left( \frac{1}{\sqrt{u^2 - 1}} \right)} - 1 \right)}{\epsilon} \right],
\]

where \( u = \frac{\epsilon}{\Delta(e)} \), \( \epsilon = eV \), which yields

\[
\frac{1}{R_N} \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta^2(e)}} \left( \frac{\text{Re} \Delta(e)}{\text{Re} \Delta(e)} \right),
\]

\[
\left( \frac{dI}{dV} \right)_{\text{dis}} (eV) = \frac{1}{R_N} \left( 1 + \frac{\epsilon + \Delta(e)}{2e^2} - \frac{\epsilon + \Delta(e)}{2e^2} \right),
\]

It is well known that in the tunnel regime the differential conductance is proportional to the quasiparticle density of states [1]:

\[
\left( \frac{dI}{dV} \right)_{\text{tun}} (eV) = \frac{1}{R_N} \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta^2(e)}}, \quad \epsilon = eV.
\]

We assume \( T = 0 \) in these formulae, but they can be generalized to a finite temperature as well.

These formulae acquire a very simple form in the limit \( eV \gg \Delta \). For tunnel, ballistic and diffuse point contacts they are as follows:

\[
\left( \frac{dI}{dV} \right)_{\text{tun}} (eV) = \frac{1}{R_N} \left[ 1 + \frac{\epsilon + \Delta(e)}{2e^2} - \frac{\epsilon + \Delta(e)}{2e^2} \right],
\]

\[
\left( \frac{dI}{dV} \right)_{\text{bal}} (eV) \approx \frac{1}{R_N} \left[ 1 + \frac{\epsilon + \Delta(e)}{4e^2} + \frac{\epsilon + \Delta(e)}{4e^2} \right],
\]

and

\[
\left( \frac{dI}{dV} \right)_{\text{dis}} (eV) \approx \frac{1}{R_N} \left[ 1 + \frac{\epsilon + \Delta(e)}{3e^2} \right],
\]

where \( \epsilon = eV \), respectively. Thus, the \( dI/dV \)-characteristics of any point contact (tunnel, ballistic, diffusive) are roughly similar below 80 meV, where the contribution of \( \text{Im} \Delta(e) \) is negligible.

In order to compare the theoretical predictions with the experimental spectra we express the calculated spectra as the second harmonic (i.e., \( \text{rms} \) voltage, \( V_2(V) \)) of the small first harmonic modulation voltage \( V_1 \) by expanding the \( V(I) \) characteristic in the Taylor series. Namely, we express the \( V_2 \)-signal as

\[
V_2(V) \approx \frac{V_1^2}{2\sqrt{2} d} \left( R_N \frac{dI}{dV} \right),
\]

assuming that changes in differential resistance is small and, correspondingly, the modulation voltage is fixed at \( V_1 \). Any other spectra can be reduced to the particular value of \( V_1 \) using the equation [8]. In what follows we choose \( V_1 = 3 \text{ meV} \), which is close to the value used in the experiments.

In Fig. (a), (b) the calculated by formulae [5], [6], [7], and [8] second harmonic voltages \( V_2(V_1 = 3 \text{ meV}) \).
are shown for the $\pi-$ and $\sigma-$bands of MgB$_2$. These extreme regimes of current flow: tunnel, ballistic, and diffusive, are calculated using $\Delta(eV)$ functions from Fig. 4. One can see a small amplitude (of the order of 1 $\mu V$) of the phonon structure for the $\pi-$band, and a much stronger $E_{2g}$ phonon mode singularity at about 80 meV for the $\sigma$-band. Up to $eV \approx 80$ meV the self-energy structure is determined by $\text{Re}\Delta(\epsilon)$. The amplitude of phonon structure is different, reflecting the corresponding prefactors $1/2 \rightarrow 1/3 \rightarrow 1/4$ in the row of current flow regimes: tunnel $\rightarrow$ diffusive $\rightarrow$ ballistic. On the other hand, large differences in shape are observed in the energy range 80÷120 meV, where $\text{Im}\Delta(\epsilon)$ becomes appreciable. We shall see below that just at the high energy edge the experimental curves show some variation due to the uncontrollable changes of scattering in the contact region.

Comparison with experiment.

Since the theoretical spectra are odd with regard to the changes of the $dc$ voltage sign, we extract the odd part of the raw data as shown in Fig. 3:

$$V_{2,\text{odd}} = \frac{1}{2}[V_2(eV) - V_2(-eV)].$$

In Fig. 4 we compare 3 odd parts of the experimental spectra for different point-contacts which are perpendicular to the surface of the $c$-oriented thin film [13]. The superconducting energy gaps $\Delta_0$ measured by the Andreev reflection spectroscopy from $dV/dI$-characteristic lie in the range 2.1÷2.6 meV. These $dV/dI$-curves show almost no traces connected with the large gap at about 7 meV. Hence, for this orientation we probe only the $\pi$-band [3]. We compare the experimental curves (Fig. 4 (a)) with the $\pi$-band calculated spectra (Fig. 4 (b)), since in the experiments the regime of current flow is among the extremes calculated by the theory. One can see that not only the shape of the experimental spectra corresponds well to the theoretical ones (with minor deviations), but also the amplitude of the structure has a proper order of magnitude ($\sim 0.1\%$ of $R_N$). From the $dV/dI(V)$Andreev reflection spectra (see the caption in Fig. ??) one can suggest that our contacts are closer to the tunnel regime in the series of the experimental curves with resistances $49 \rightarrow 36 \rightarrow 80$ $\Omega$. To make the estimation more quantitative, one needs an interpolation formula similar to the finite barrier parameter $Z$ in the BTK-theory [14].

The question arises as to why we did not observe a much stronger self-energy S-type-structure in Ref. [15], where the point-contact spectrum of MgB$_2$ single crystal was measured along $ab$-plane? The answer is that in that case the nonequilibrium phonon generation is so strong that superconductivity in the contact region is destroyed, and correspondingly, the excess current dramatically decreases around the $E_{2g}$ phonon mode energy. This leads to a large maximum in the $dV/dI(V)$ characteristic and the N-shape singularity in $V_2(V)$. The maximum can be
FIG. 4: Comparison of three different experimental point-contact spectra (panel (a)) in the c-direction (Ref. [7]) with the theoretical ones (panel (b)) calculated by asymptotic formulae (5), (6), (7), and (8) based on superconducting order parameter $\Delta(\epsilon)$ from Fig. 1. All the curves are displaced vertically for clarity and reduced to modulation voltage $V_1 = 3$ mV. In panel (a), the normal state resistances 49 and 36 $\Omega$ correspond to zero-bias $R_0 = 45$ and 43 $\Omega$, respectively, being the same as in Fig. 2 (b) of Ref. [7]. For $R_N = 80$ $\Omega$ $R_0 = 150$ $\Omega$. The experimental curves are smoothed by several mV not disturbing the phonon structure. $T=4.2$ K, $H=0$.

easily seen in the $V_1(V)$-characteristic (note, for example, the inset in Fig. 1 of Ref. [13]). Normally, this destruction of superconductivity masks the self-energy structure effectively. It can be identified by the strong dependence of energy position on external parameters: magnetic field and temperature.

Summary.

In conclusion, we have derived the simple asymptotic formulae for the order parameter self-energy effects in the superconducting point-contact. They can be used in standard programs [16, 17] to solve the Eliashberg equations [4] for quantitatively derivation of electron-phonon-interaction spectral function providing the structure of point-contact is established. In MgB$_2$, we applied them in c-direction for obtaining point-contact spectra in $\pi$-band. The close similarity between the calculated and measured point-contact spectra in the c-direction manifests the validity of the calculated EPI spectral function in the $\pi$-band in Ref. [10].

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