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The determination of the electron–phonon interaction from tunneling data in the two-band superconductor MgB_2

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Abstract

We calculate the tunneling density of states (DOS) of MgB_2 for different tunneling directions, by directly solving the real-axis, two-band Eliashberg equations (EE). Then we show that the numeric inversion of the standard single-band EE, if applied to the DOS of the two-band superconductor MgB_2, may lead to wrong estimates of the strength of certain phonon branches (e.g. the E_{2g}) in the extracted electron–phonon spectral function $\alpha^2F(\omega)$. The fine structures produced by the two-band interaction turn out to be clearly observable only for tunneling along the *ab*-planes in high-quality single crystals. The results are compared to recent experimental data.

Keywords: Electron–phonon interaction; Eliashberg equations; Magnesium diboride

There is a growing consensus that superconductivity in MgB_2 is driven by the electron–phonon interaction (EPI) [1]. The idea of multiband superconductivity in MgB_2 [2–5] is supported by many recent experimental results from tunneling [6,7], point contact [8,9] and specific heat measurements [10]. These data give direct evidence that the superconducting gap has two different values: Δ_σ for the two quasi-two-dimensional σ bands, and Δ_π for the 3D π bands [2,3]. According to most calculations [2,4,11], the EPI or, equivalently, the Eliashberg spectral function $\alpha^2F(\omega)$ (EF) is dominated by the optical boron bond-stretching E_{2g} phonon branch around 60–70 meV.

At present, the main experimental tool for the determination of the EPI in superconductors is tunnel spectroscopy. Unfortunately, the standard single-band procedure to obtain the EF from the first derivative of the tunneling current is restricted to a momentum-independent s-wave order parameter and cannot be used in anisotropic superconductors like MgB_2. Nevertheless, there has been a recent attempt to obtain the EPI in MgB_2 by using this standard approach [12].

In the present paper we clarify what information can be obtained by using this *single-band* standard procedure if one applies it to a *two-band* superconductor.

The parameters for the two-band model used in this work are based on first-principle electronic structure calculations [11]. The four interband and intraband electron–phonon spectral functions $\alpha^2F_{ij}(\omega)$ (where $i,j = \pi,\sigma$) and the Coulomb pseudopotential matrix μ^*_{ij} are the basic input for the two-band Eliashberg theory. The $\sigma\sigma$ EPI is dominated by the optical boron bond-stretching E_{2g} phonon mode. For the other channels there are also important contributions from low-frequency (30–40 meV) and from high-frequency phonon modes ($\approx$90 meV).

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We obtained the theoretical conductance curves of MgB_2 for different tunneling directions by solving the corresponding two-band Eliashberg equations (EE) [3,13] in the real-axis formulation. The only free parameter is the normalization constant μ in the Coulomb pseudopotential matrix which is fixed in order to reproduce the experimental $T_c = 39.4$ K. Fig. 1(a) and (b) show the calculated conductances for tunneling along the *ab*-plane and the *c*-axis directions, respectively. According to Ref. [3], these conductances are a weighed sum of the σ- and π-band contributions to the DOS, whose weights w_σ and w_π are determined by the corresponding Fermi velocities in the bands and by the angle of the tunneling current with respect to the *ab*-plane. The values of these weights are $w_\sigma = 0.33$ and $w_\pi = 0.67$ for tunneling along the *ab*-plane, $w_\sigma = 0.01$ and $w_\pi = 0.99$ for tunneling along the *c*-axis. It is clear that the contribution of the π band is always dominant even if tunneling is almost in the *ab*-plane. The fine structures due to the EPI have maximum amplitudes of the order of 0.5% and 2–3% for measurements along the *c*-axis and in the *ab*-plane, respectively (see the two insets of Fig. 1).

In order to test the reliability of the numeric inversion of the standard *single-band* Eliashberg equations when applied to a *two-band* superconductor, we used the calculated tunneling DOS shown in Fig. 1 as an input. Of course, in this case, the inverted spectral function should correspond to a mixture of the σ- and π-band contributions. Fig. 2(a) and (b) show the results of the inversion of the calculated tunneling DOS of Fig. 1(a) and (b), respectively, using a standard single-band code (solid lines). The effect of the single-band EE inversion is estimated by a least-square fit of the inverted spectral functions with the weights for $\alpha^2F_\sigma = \alpha^2F_{\sigma\sigma} + \alpha^2F_{\sigma\pi}$ and $\alpha^2F_\pi = \alpha^2F_{\pi\pi} + \alpha^2F_{\pi\sigma}$ as free parameters. These fits are shown by the dashed curves in Fig. 2 and correspond to $\alpha^2F_{ab}^{\mathrm{fit}} = 0.31\alpha^2F_\sigma + 0.16\alpha^2F_\pi$ and $\alpha^2F_c^{\mathrm{fit}} = 0.01\alpha^2F_\sigma + 0.99\alpha^2F_\pi$.

Tunneling along the *c*-direction practically corresponds to a single-band case and, as expected, the inversion properly reproduces the α^2F_π. In contrast, in the case of tunneling along the *ab*-direction, the σ-band spectral functions play an essential (and amplified) role since about 33% of the σ-band contribution in the tunneling DOS corresponds to a contribution of about 66% of α^2F_σ in the effective α^2F_{ab}.

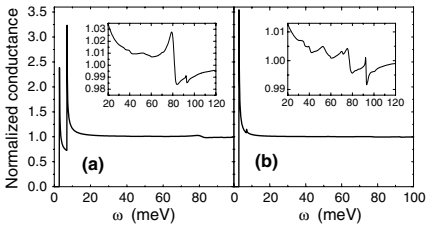

Fig. 1. The calculated tunneling DOS at $T = 0$ K in the *ab*-plane (a) and along the *c*-axis (b). The two insets show the fine structures of the tunneling DOS due to the electron–phonon interaction.

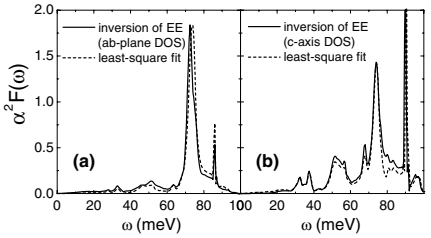

Fig. 2. The Eliashberg functions for tunneling along the *ab*-plane (a) and along the *c*-axis (b) obtained from the curves of Fig. 1 by inversion of the single-band Eliashberg equations (solid line). The dashed lines represent the least-square fits with two free parameters as explained in the text.

The above results show that, in polycrystalline samples and in non-oriented films (where the π band dominates the tunneling current), the inversion of the experimental DOS gives mainly information about $\alpha^2F_\pi(\omega)$, and thus leads to underestimate the strength of the E_{2g} phonon mode that is essential for superconductivity. This might explain the results reported in Ref. [12], where the dominant role of the E_{2g} phonon mode was questioned. Thus, only separate studies of very low-temperature *ab*-plane and *c*-axis tunneling conductances in high-quality single crystals in clean limit might allow a quantitative estimate of the EPI. These studies should provide a crucial test for the results of the two-band model, even though the fine structures in the DOS due to the EPI are very likely to be experimentally observable only for tunneling current parallel to the *ab*-planes.

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