Extraction of the electron-phonon interaction from tunneling data in the multigap superconductor MgB_2

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The direct inversion of the Eliashberg equations (EE) in case of a multiband superconductor is a mathematically ill-defined problem, because it is not possible to obtain several band splitted electron-phonon spectral functions $\alpha^2F_{ij}(\omega)$ from a single function of the tunnel current. In the present work we follow another direction and calculate the tunneling density of states (DOS) of MgB_2 for different tunneling directions by directly solving the two-band EE in the real-axis formulation. This procedure reveals the fine structures of the DOS due to the optical phonons. Then we show that the numeric inversion of the standard *single-band* EE, when applied to the *two-band* DOS of MgB_2, underestimates the strength of certain phonon branches (e.g., the E_{2g}) in the extracted $\alpha^2F(\omega)$. The fine structures produced by the two-band interaction at energies between 20 and 100 meV turn out to be clearly observable only for tunneling along the ab planes and at very low temperature. Only in this case it is possible to extract some information on the σ-band contribution to the spectral functions. For any other tunneling direction, the π-band contribution is dominant and almost coincides with the whole $\alpha^2F(\omega)$ for tunneling along the c axis. Our results are compared with recent experimental tunneling and point-contact data.

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There is a growing consensus that the superconductivity in MgB_2 with a critical temperature $T_c \simeq 40$ K (Ref. 1) is driven by the electron-phonon interaction (EPI) (for a recent review see Ref. 2). An important subject to address for a proper understanding of the surprising physical properties of this material is the character of the order parameter (or superconducting gap): is it constant over the whole Fermi surface, or strongly momentum dependent? The idea of multiband superconductivity in MgB_2 (Refs. 3–9) is supported by many recent experimental results from tunneling,[10–12] point contact,[13–15] and specific-heat capacity measurements.[6,16] These data directly support the picture that the superconducting gap has two different values on two qualitatively different parts of the Fermi surface, one Δ_σ for the two quasi-two-dimensional σ bands and another one Δ_π for the pair of three-dimensional (3D) π bands.[3,5]

While, within first-principles calculations of the electronic structure and the EPI in this compound, there is an agreement[17] on this qualitative picture, still disagreement is present about the precise values of characteristic frequencies and coupling constants. According to most calculations,[3,18,19,8] the EPI or, equivalently, the Eliashberg spectral function $\alpha^2F(\omega)$ (EF) is dominated by the optical boron bond-stretching E_{2g} phonon branch of around 60–70 meV.

In principle, photoemission lineshapes or the deviation of the far-IR absorption from the Drude law are controlled by the same Eliashberg functions as tunneling or their transport counterparts, so that optical measurements can also deliver information on the EPI.[20,21] Unfortunately, the extraction of the spectral functions from these experiments, for a variety of reasons, is technically much more challenging than from tunneling data. Therefore, the main experimental tool for the determination of the EPI in superconductors so far is the tunneling measurement. This method has been applied to standard superconductors with an isotropic (constant in **k** space) superconducting gap and allowed for the determination of the Eliashberg spectral functions in the case of many conventional low-temperature superconductors (see, e.g., Ref. 22).

The spectral function is obtained from the first derivative of the tunneling current

$$\frac{dI_T}{dV} \propto N^T = \alpha_T \mathrm{Re} \frac{E}{\sqrt{E^2-\Delta^2(E)}}\bigg|_{E=eV}, \qquad (1)$$

where V is the applied voltage, $\Delta(E)$ is the *complex* superconducting gap which depends on energy E, and the factor α_T is determined by the properties of the tunneling barrier and the corresponding average of the Fermi velocities of quasiparticles. The standard single-band procedure to obtain the EF from the tunneling DOS can be found in textbooks.[22,23] Another mathematically elegant method has been proposed in Ref. 24. It has been used to investigate conventional (low T_c) as well as high-temperature superconductors.[25]

Unfortunately, this approach is restricted to momentum independent *s*-wave order parameters and cannot be used to describe anisotropic superconductors as MgB_2. In fact, tunneling experiments produce a single function $I(V)$ but in the framework of the two-gap model we have to determine from this single function $I(V)$ the three spectral functions

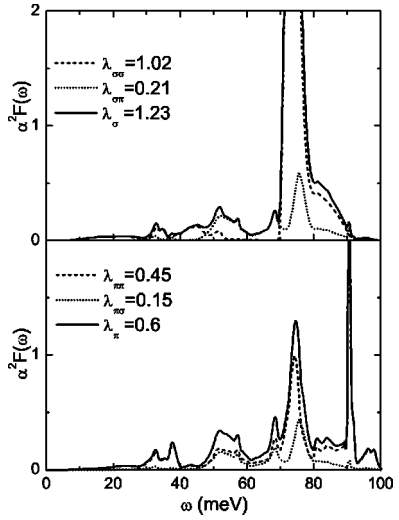

FIG. 1. The theoretical Eliashberg spectral functions of MgB_2 for the two-band model used in this work (from Ref. 6). The thick solid lines correspond to the total σ- and π-band contributions.

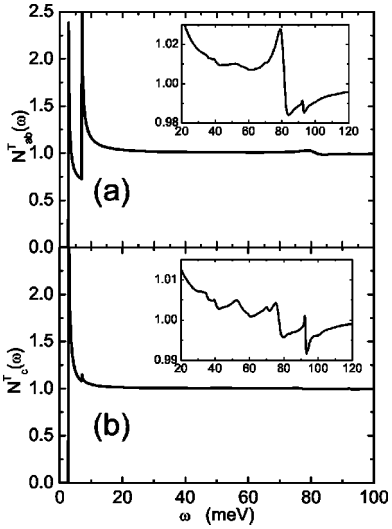

FIG. 2. (a) The calculated tunneling DOS in the ab plane; (b) the calculated tunneling DOS along the c axis. They are both obtained by the real-axis solution of the two-band Eliashberg equations at $T=0$ K. The two insets show the fine structures of the tunneling DOS due to the electron-phonon interaction.

$\alpha^2F_{\sigma\sigma}(\omega)$, $\alpha^2F_{\sigma\pi}(\omega)$ and $\alpha^2F_{\pi\pi}(\omega)$ (the function $\alpha^2F_{\pi\sigma}(\omega)$ is not independent), which is an impossible task. Nevertheless, there has been a recent attempt to obtain the EPI in MgB_2 by using this standard approach.[26] The E_{2g} phonon mode has been resolved, but its predominance for the electron-phonon coupling was questioned. More recently, the E_{2g} mode has been also resolved in point-contact spectra.[27]

The purpose of this paper is to clarify what information can be extracted using this *single-band* standard procedure if one applies it to a *two-band* superconductor. The starting point is the theoretical study of the quasiparticle tunneling in MgB_2-based junctions. The superconducting gap functions for the σ and π band are obtained from an extended Eliashberg formalism. The parameters for the two-band model utilized in this work, which are based on first-principles electronic structure calculations,[18] have been used before for a successful description of specific heat[6] and tunneling[7] properties of MgB_2. The interband and intra-band electron-phonon spectral functions $\alpha^2F_{ij}(\omega)$, where $i,j=\pi,\sigma$ (see Fig. 1) and the Coulomb pseudopotential matrix μ^*_{ij} (see Ref. 28) are the basic input for the two-band Eliashberg theory. The theoretical conductance curves of MgB_2 for different tunneling directions can be obtained directly by solving the corresponding two-band Eliashberg equations Eliashberg equations (EE)[7] in the real-axis formulation. In pure clean limit (i.e., by neglecting the interband scattering), 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.

One may see in Fig. 1 that the $\sigma\sigma$ EPI is dominated by the optical boron bond-stretching E_{2g} phonon mode. For other channels there are also important contributions from low frequency modes (30–40 meV) and from high-frequency phonon modes ($\simeq$90 meV). In contrast to the case of a conventional junction described by Eq. (1), the conductance in a MgB_2-I-N tunnel junction is a weighted sum of the contributions of the DOS of σ and π bands, where the weights are determined by the corresponding plasma frequencies ω_p in the bands and by the angle of the tunneling current with respect to the ab plane.[7] Figure 2(a) and 2(b) shows the calculated tunneling conductances at $T=0$ K in the ab plane and along the c-axis direction. In the case of MgB_2 according to Ref. 7,

$$N^T_{ab}(\omega)=\frac{(\omega^{\sigma}_{\mathrm{p,ab}})^2}{(\omega^{\mathrm{tot}}_{\mathrm{p,ab}})^2}N_{\sigma}(\omega)+\frac{(\omega^{\pi}_{\mathrm{p,ab}})^2}{(\omega^{\mathrm{tot}}_{\mathrm{p,ab}})^2}N_{\pi}(\omega),$$

$$N^T_{c}(\omega)=\frac{(\omega^{\sigma}_{\mathrm{p,c}})^2}{(\omega^{\mathrm{tot}}_{\mathrm{p,c}})^2}N_{\sigma}(\omega)+\frac{(\omega^{\pi}_{\mathrm{p,c}})^2}{(\omega^{\mathrm{tot}}_{\mathrm{p,c}})^2}N_{\pi}(\omega), \qquad (2)$$

where $N_{\sigma}(\omega)$ and $N_{\pi}(\omega)$ are the partial superconducting DOS, and the numerical values of the squares of the ratio of the plasma frequencies are 0.33 (0.67) for σ (π) in the ab plane and 0.01 (0.99) for σ (π) in the c direction according to Table I of Ref. 7. The contribution of the π band is always dominant even if tunneling is almost in the ab plane.[7] In the insets of Fig. 2 the fine structures due to electron-phonon interaction are shown. The maximum amplitude of these structures at very low temperature is of the order of 0.5% for measurements along the c axis and 2–3% in the ab plane. The double-gap features of the DOS visible in the ab plane $N^T_{ab}(\omega)$ should be experimentally observable even for a certain amount of impurity scattering because the interband impurity scattering rate appears to be very weak.[9] On the other hand, due to the smallness of the σ-band plasma frequency in the c direction, the conductance in the c-axis direction is almost totally determined by the π band and therefore no double-peak structure is expected in the conductance spectrum. In fact this change in behavior has been experimentally observed by spatially well-defined tunnel measurements over

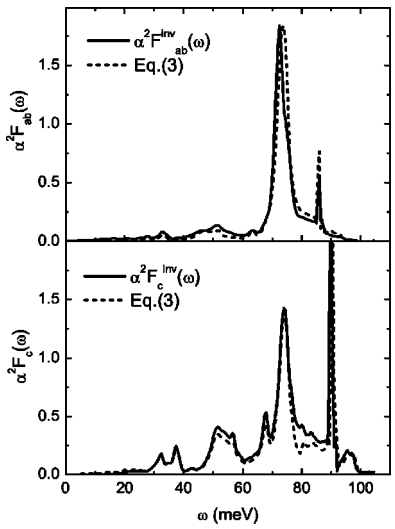

FIG. 3. The spectral Eliashberg functions along the ab plane (upper panel) and along the c axis (lower panel) obtained by inversion of the single-band Eliashberg equations (solid line) applied to the tunneling DOS of Fig. 2. The dashed lines represent the least-square fits of these spectral functions with two free parameters for α^2F_σ and α^2F_π as explained in the text.

a step edge in small MgB_2 single crystals[11] and by directional point-contact spectroscopy in larger crystals.[15]

In order to test the reliability of the numeric inversion technique of the standard *single-band* Eliashberg equation when applied to a *two-band* superconductor, we use the calculated tunneling DOS shown in the insets of Fig. 2 as an input. Following the standard approach we calculate the reduced density of states (N/N_{BCS})-1 and introduce it in the standard single-band inversion code starting from an energy of 15 meV, which roughly corresponds to the lowest optical phonon energy. In our case, where the DOS has been theoretically calculated, it is very easy to demonstrate that the starting point in energy for the reduced density of states (provided it is larger than the gaps) does not affect the final results.[29]

Of course, in the case of a single-band superconductor the inversion should reproduce the shape of the single-band Eliashberg function used for the calculation of the tunneling DOS. This will not be true anymore if one tries to invert a tunneling DOS which is derived from a multiband Eliashberg theory. The inverted spectral functions should correspond to the mixture of the σ- and π-band contributions. We can introduce the following functions:

$$\alpha^2F_\sigma(\omega)=\alpha^2F_{\sigma\sigma}(\omega)+\alpha^2F_{\sigma\pi}(\omega),$$

$$\alpha^2F_\pi(\omega)=\alpha^2F_{\pi\pi}(\omega)+\alpha^2F_{\pi\sigma}(\omega).$$

Namely, these functions determine the normal state properties in the two-band model. Tunneling measurements can only give information on these combinations of $\alpha^2F_{i,j}(\omega)$ $(i,j=\sigma,\pi)$ which are indicated by thick lines in Fig. 1. In order to illustrate this point we show in Fig. 3(a) and 3(b) the results of the inversion of our calculated tunneling DOS shown in the insets of Fig. 2(a) and 2(b) using a standard single-band code[24] (solid lines). The effect of the single-band EE inversion is estimated by a least-square fit to the inverted spectral functions with the weights for α^2F_σ and α^2F_π as free parameters. These fits are shown by the dashed curves in Fig. 3. Since tunneling along the c direction—due to the very different plasma frequencies in the two bands[7]—practically corresponds to a single-band case, the inversion properly reproduces the α^2F_π as one expects. In contrast, in the case of tunneling along the ab direction (which corresponds to an actual multiband situation) the weights are quite different from the theoretical expectation. The results of this particular fit are summarized below:

$$\alpha^2F_{ab}(\omega)\simeq 0.31\alpha^2F_\sigma(\omega)+0.16\alpha^2F_\pi(\omega),$$

$$\alpha^2F_c(\omega)\simeq 0.01\alpha^2F_\sigma(\omega)+0.99\alpha^2F_\pi(\omega). \qquad (3)$$

As one may see the σ-band spectral functions $\alpha^2F_{\sigma\sigma}(\omega)+\alpha^2F_{\sigma\pi}(\omega)$ play an essential (and amplified) role only if the contribution of $N^T_\sigma(\omega)$ is significant. The numerical simulations show that about 33% of the σ-band contribution in the tunneling DOS corresponds to a contribution of about 66% of $\alpha^2F_\sigma(\omega)$ in the effective $\alpha^2F_{ab}(\omega)$. These results are reasonable since $\lambda_\pi=(\lambda_{\pi\pi}+\lambda_{\pi\sigma})\approx 0.6$ while $\lambda_\sigma=(\lambda_{\sigma\sigma}+\lambda_{\sigma\pi})\approx 1.23$. Somewhat simplifying it seems that the contributions of the tunneling DOS to the phonon structures are weighted by the corresponding coupling constants. The inversion of the c-axis case results in a $\alpha^2F_c(\omega)$ that is almost exactly the sum of the $\alpha^2F_i(\omega)$ components taken with the same weights present in the sum of the corresponding superconducting $N^T_\pi(\omega)$ and $N^T_\sigma(\omega)$ (see, Eq. (2)). In this case, the coupling constant from the inversion is almost equal to λ_π, and therefore the effective Eliashberg function will show strong contributions from low- and high-frequency phonons.

In order to check how much these results depend on the shape of the $\alpha^2F_{i,j}(\omega)$, we performed all the previous calculations by using some Lorentzian peaks with the same integrated coupling strength as the first-principles spectral functions. In this case the results of the single-band inversion show the same general features described in Eq. (3) even if the coefficients are somehow different: the π-band contribution is always dominant for tunneling along the c direction, while the σ-band one is the greatest for tunneling along ab planes.

The above results show that from tunneling measurements at very low temperatures, and by numeric inversion of the standard single-band Eliashberg equations, one can obtain reliable information on the EPI in MgB_2 only for the π band. To do this, we can use the Donetsk's inversion program[24] that allows finding the $\alpha^2F(\omega)$ for a single-band superconductor.

The interesting point is that from tunneling measurements exactly along ab and c directions on single crystals in the clean limit it should be possible to extract information on $\alpha^2F_\pi(\omega)$ and $\alpha^2F_\sigma(\omega)$. This could be a useful method to test the two-band model and identifying the phonon modes responsible for superconductivity in MgB_2. Nevertheless, from the experimental point of view, this possibility could

remain only virtual since the smallness of the phonon structures expected in the tunneling along the *c* axis [see the inset of Fig. 2(b)] and the thermal broadening present even at temperatures of the order of 2–4 K could prevent a correct inversion of the EE in the presence of noise. We calculated that already at 5 K the ab plane phonon structures are so smeared that the inverted spectral function strongly underestimates the role of the E_{2g} phonon mode.

In polycrystalline samples the π band dominates the tunneling current[7] and it is only possible to extract information about the combination of spectral functions $\alpha^2F_\pi(\omega)$, which does not play an important role for the superconducting properties of MgB_2. The recent work of D'yachenko *et al.*,[26] which claims the experimental determination of $\alpha^2F(\omega)$, is very likely contaminated by strong contributions from the π band and by the thermal broadening. Unfortunately, such data cannot give information on the nature of superconductivity in a two-band superconductor such as MgB_2 which is driven by the interaction in the σ band. A similar attempt to analyze the phonon spectrum from the optical data in the frame of the single-band model has been made in Ref. 30.

In conclusion, only in junctions with the tunneling current running along the ab planes and at very low temperature one can observe the fine structures of the superconducting DOS produced by the electron-phonon interaction at energies between 20 and 100 meV. In recent point-contact measurements[27] the anisotropic EPI was observed, though no quantitative estimate was presented. Further experiments on high-quality tunnel junctions are needed in order to obtain data allowing for a quantitative estimate of the EPI, which should also take into account the 'tunneling cone' effect,[22] i.e., the distribution of tunneling angles. Since the direct inversion approach is not possible we propose here to attack the problem from another direction. Using Eliashberg spectral functions from first-principles calculations as an input and calculating the tunneling DOS from the solution of the Eliashberg equations for different tunneling directions a direct comparison with experiments becomes possible. According to our result, separate studies of ab-plane and *c*-axis tunneling conductances from data at very low temperature in high-quality single crystals may allow a quantitative estimate of the EPI and should thus provide a crucial test for the first-principle results of the two-band model.

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