Can one extract the electron-phonon-interaction from tunneling data in case of the multigap superconductor MgB$_2$?

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In the present work we calculate the tunneling density of states (DOS) of MgB$_2$ for different tunneling directions by directly solving the two-band Eliashberg equations (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 (the only available method), when applied to the two-band DOS of 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 $\alpha^2 F(\omega)$. 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, when the extracted $\alpha^2 F(\omega)$ contains the combination $\alpha^2 F_{\sigma}(\omega)+\alpha^2 F_{\pi}(\omega)$, together with a minor $\alpha^2 F_{\sigma}(\omega)+\alpha^2 F_{\pi}(\omega)$ component. Only in this case it is possible to extract information on the $\sigma$-band contribution to the spectral functions. For any other tunneling direction, the $\pi$-band contribution (which does not determine the superconducting properties of MgB$_2$) is dominant and almost coincides with the whole $\alpha^2 F(\omega)$ 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 superconductivity in MgB$_2$ with a critical temperature $T_c \approx 40 K$ (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$_2$ is supported by many recent experimental results from tunneling$^{13,14,15,16,17}$, point contact$^{15,16,17}$ and specific heat capacity measurements$^{18}$. These data directly support the picture that the superconducting gap has two different values on two qualitatively different parts of the Fermi surface, one $\Delta_{\sigma}$ for the two quasi-two-dimensional $\sigma$ bands and another one $\Delta_{\pi}$ for the pair of 3D $\pi$ bands$^{3,5}$.

While, within first-principles calculations of the electronic structure and the EPI in this compound, there is an agreement$^{13,14,15,16,17}$ on this qualitative picture, still disagreement is present about the precise values of characteristic frequencies and coupling constants. According to most calculations$^{13,14,15,16,17}$, the EPI or, equivalently, the Eliashberg spectral function $\alpha^2 F(\omega)$ (EF) is dominated by the optical boron bond-stretching $E_{2g}$ phonon branch around 60 - 70 meV.

In principle, photoemission or optical measurements can also deliver information on the EPI$^{13,14,15,16,17}$, although 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 $\mathbf{k}$-space) superconducting gap and allowed for the determination of the Eliashberg spectral functions in case of many conventional low-temperature superconductors (see e.g. Ref. $^{22}$).

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

$$
\frac{dI}{dV} \propto N_T = \alpha_T \text{Re} \frac{E}{\sqrt{E^2 - \Delta^2(E)}} \bigg|_{E=E_F},
$$

where $V$ is the applied voltage, $\Delta(E)$ is the complex superconducting gap which depends on energy $E$, and the factor $\alpha_T$ 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$^{24}$.

Unfortunately, this approach is restricted to momentum independent $s$-wave order parameters and cannot be used to describe anisotropic superconductors as MgB$_2$. Nevertheless, there has been a recent attempt to obtain the EPI in MgB$_2$ by using this standard approach$^{25}$. The $E_{2g}$ phonon mode has been resolved, but its predominance for the electron-phonon coupling was questioned. More recently, the $E_{2u}$ mode has been also resolved in point-contact spectra$^{25}$.

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 $\sigma$ and $\pi$ 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, have been used before for a successful description of specific heat and tunneling properties of MgB$_2$. The interband and intraband electron-phonon spectral functions $\alpha^2 F_{ij}(\omega)$, where $i,j = \pi, \sigma$ (see Fig. 1) and the Coulomb pseudopotential matrix $\mu_{ij}^c$ (see Ref. 20) 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 (EEs) in the real-axis formulation. The only free parameter is the normalization constant $\mu$ 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 $\sigma$ and $\pi$ bands, where the weights are determined by the corresponding Fermi velocities (plasma frequencies) in the bands and by the angle of the tunneling current with respect to the $ab$ plane. Figure 2 (a) and (b) shows the calculated tunneling conductances in the $ab$-plane and along the $c$-axis direction. In the case of MgB$_2$ according to Ref. 20,

$$
N_{\sigma\sigma}^T(\omega) = 0.33 N_\sigma(\omega) + 0.67 N_\pi(\omega),
$$

$$
N_{\pi\pi}^T(\omega) = 0.01 N_\sigma(\omega) + 0.99 N_\pi(\omega),
$$

where $N_\sigma(\omega)$ and $N_\pi(\omega)$ are the partial superconducting DOS.

The contribution of the $\pi$ band is always dominant even if tunneling is almost in the $ab$ plane. In the insets of Fig. 2 the fine structures due to electron-phonon interaction are shown. The maximum amplitude of these structures is of the order of 0.5% for measurements along the $c$-axis and 2-3% in the $ab$-plane. The double-gap fea-

FIG. 1: The theoretical Eliashberg spectral functions of MgB$_2$ for the two-band model used in this work (from Ref. 10). The thick solid lines correspond to the total $\sigma$- and $\pi$-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.
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 $\sigma$- and $\pi$-band contributions. We can introduce the following functions:

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

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

Namely, these functions determine the normal state properties in the two-band model. Tunneling measurements can only give information on these combinations of $\alpha^2 F_{i,j}(\omega)$ ($i, j = \sigma, \pi$) which are indicated by thick lines in Fig. 1. In order to illustrate this point we show in Figure 3 (a) and (b) the results of the inversion of our calculated tunneling DOS of Fig. 2 (a) and (b) using a standard single-band code (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 $\alpha^2 F_{\sigma}$ and $\alpha^2 F_{\pi}$ 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— practically corresponds to a single-band case, the inversion properly reproduces the $\alpha^2 F_{\pi}$ 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 the fit are summarized below:

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

$$
\alpha^2 F_{\pi}(\omega) \simeq 0.01 \alpha^2 F_{\sigma}(\omega) + 0.99 \alpha^2 F_{\pi}(\omega)
$$

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

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 $\pi$ band. For doing this we can use the Donetsk’s inversion program which allows to find the $\alpha^2 F(\omega)$ for a single-band superconductor.
The interesting point is that measuring single crystals in the clean limit one should see different phonon contributions for different tunneling directions, in accordance with the two-band model. From tunneling measurements exactly along \(ab\) and \(c\) directions it is possible to extract information on \(\alpha^2 F_\nu(\omega)\) and on \(\alpha^2 F_{ab}(\omega)\), by solving the system of equations (3) and this could be a useful method for testing the two-band model and identifying the phonon modes responsible for superconductivity in MgB\(_2\). From the experimental point of view this possibility could only remain virtual since the smallness of the phonon structures expected in the tunneling along the \(c\) axis (see the inset of Fig. 2 (b)) could prevent a correct inversion of the EE in the presence of noise. In polycrystalline samples the \(\pi\) band dominates the tunneling current and it is only possible to extract information about the combination of spectral functions \(\alpha^2 F_{\nu}(\omega)\), which does not play an important role for the superconducting properties of MgB\(_2\). The recent work of D’yachenko et al.\(^\text{20}\) which claims the experimental determination of \(\alpha^2 F(\omega)\), is very likely contaminated by strong contributions from the \(\pi\) band. A value of the coupling constant \(\lambda = 0.9\) was reported in Ref.\(^\text{20}\). Unfortunately, such data cannot give information on the nature of superconductivity in a two-band superconductor as MgB\(_2\) which is driven by the interaction in the \(\sigma\) band.

The inversion of the calculated \(ab\)-plane conductance \(N_{ab}(\omega)\) shows that a significant contribution to the phonon structures comes from \(\sigma\) bands and this is reflected in the resulting \(\alpha^2 F_{ab}(\omega)\). Therefore, only in junctions with the tunneling current running along the \(ab\) planes and at 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\(^\text{22}\) 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, i.e. the distribution of tunneling angles. According to our result shown in Eq. (3) separate studies of \(ab\)-plane and \(c\)-axis tunneling conductances 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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