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Two band superconductivity in Eliashberg model for MgB_2

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The superconductivity in MgB_2 is analyzed inside a two band model. The model consists in self-consistent calculation of the gap and effective mass renormalization functions of Eliashberg equations. We present the frequency dependence of the two functions, and the temperature dependence of the two energy gaps, revealing the superconducting transition temperature T_c. The results show the role of the strong electron – phonon coupling in superconductivity of MgB_2 via high frequency phonons of E_{2g} mode. The superconductivity mainly originates in the quasi *2D* σ band, being driven from interaction inside the boron layer. The out of plane interaction is weaker and the *3D* π band has a smaller contribution to superconductivity.

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1. Introduction

Since the discovery of the superconducting transition in MgB_2 [1], the high value of the critical temperature, T_c ~ 39 K, the highest ever achieved for a binary compound and above the theoretical predicted value from *BCS* theory [2], was the starting point for an intense dispute in scientific community. The main problem which required an answer was if this compound should be considered as a "classical" superconductor, or as a new type of high temperature superconductor (*HTS*). A large amount of experiments [3] suggests that strong electron – phonon interaction is the adequate mechanism which describes its superconductivity. For understanding this mechanism, it's important to briefly analyze the spatial and band structure of this compound. The spatial structure of MgB_2 is a simple hexagonal layered structure ($P6/mmm$ space group), consisting of hexagonal graphite-type boron layers, separated by hexagonal layers of magnesium, such a layered structure being close to the structure of high-T_c cuprates. Its electronic structure is similar to that of the graphite. As determined from band calculations [4], the main contribution to the superconductivity is due to the boron, arising from the two incomplete filled of bonding-type σ bands, due to in-plane (in boron layer) sp^2 ($sp_x p_y$) hybridization, and two π bands of bonding and respectively antibonding types, due to the aromatically hybridization of the boron p_z orbitals.

Useful information regarding the band structure was obtained from the investigation of the Fermi surface in *ARPES* [5] and de Haas-van Alphen effect [6] experiments. The large in-plane overlaping of the p orbitals compared with the interlayer overlaping leads to a strong in-plane dispersion and a smaller one out of boron layer, consisting in a very small k_z dispersion of the σ bands. This weak dispersion give rise to Fermi surface sheets associated to the unfilled σ bands, hole-type, nearly cylindrical around $\Gamma - A$ direction in BZ. In contrast, the π bands correspond to the two planar tubular networks of Fermi surface sheets: an antibonding, electron-type sheet, centered at $k_z = 0$ and a bonding, hole-type sheet, centered at $k_z = \pi / c$ [7]. The sp^2 hybridization in boron layer leads to a strongly covalent bonding and the holes from the top of σ bands are localized within the layer, having a $2D$ character. In contrast, the electrons and holes from π bands are delocalized over the entirely crystal, having a $3D$ metallic-type behavior. As consequence of the coexistence of the two types of conducting bands, the total *DOS* at Fermi level consists in a sum of contributions originated in the every bands. The cylindrical (*2D* covalent bonding) and tubular (*3D* metallic bonding) sheets of Fermi surface contribute about 42% and 58% respectively, in a ratio $N_\sigma / N_\pi \cong 0.73$ [8].

A major challenge in the study of superconductivity in MgB_2 was the investigation of which of single, or two bands mechanism is implied in superconducting transition. For this purpose, the existence of a single or two energy gaps was investigated in a large amount of experiments. Some earlier experiments, as Scanning Tunneling

Spectroscopy (STS) [9,10], Far Infrared Transmission ($FIRT$) [11], Raman Spectroscopy (RS) [12], High Resolution Photoemission Spectroscopy ($HRPS$) [13], or Point Contact Tunneling Spectroscopy (PCS) [14] have proved the existence of a single energy gap of magnitude between $2.5 \div 5$ meV. Other experiments as STS [15-17], PCS [18], $HRPS$ [19], RS [20] or specific heat measurements [21,22] claimed the necessity of admitting two energy gaps for explanation the results. All these experiments together with the high isotopic effect due to the boron, confirm that in MgB_2, the appearance of superconductivity is due to the strong $s-wave$ type interaction of the pseudoparticles with phonons in intermediate, or even strong coupling [23,24]. A more recent $ARPES$ experiment [25] reports the direct experimental evidence of the two band superconductivity in MgB_2 from separately observing distinct gaps in σ and π bands of the boron. The existence of the two gaps having different magnitudes $\Delta_\sigma = 6-7meV$ and $\Delta_\pi \cong 2meV$, unambiguously established the two band nature of the superconductivity in this material. In understanding the appearance of the superconductivity, the key role is played by the pairing interaction of the quasiparticles with phonons modes described by the density of state $F(\omega)$ and Eliashberg function $\alpha^2F(\omega)$. First principle calculations for the phononic spectrum [26] showed four important phonon modes: firstly, two associated with vibrations in the Mg - Mg plane: E_{1u} ($40meV$) for vibrations in $x-y$ directions and A_{2u} ($49meV$) for vibrations in z direction, and secondly, two associated with vibrations in $B-B$ plane: E_{2g} ($67meV$) for in plane vibrations and B_{1g} ($87meV$) for in z direction, out of plane vibrations of the boron atoms. From these calculations, a sharp and narrow peak is observed in $\alpha^2F(\omega)$, at the frequency of the E_{2g} mode, leading to the result that the pairing interaction is mostly associated with the E_{2g} mode corresponding to the in boron plane vibrations. As a conclusion, the σ band with stronger electron-phonon coupling via the E_{2g} mode, associated with in-plane $B-B$ vibrations, has the dominant role, while the π band, characterized by weaker coupling with phonons corresponding to out of plane vibrations, have more minor contribution to the superconductivity, but the superconductivity originates in each band due to intra and interband processes.

2. Theoretical model

In order to describe this compound, the theoretical model should be based on the electron-phonon coupling (EPC) interaction. A two gap model, based on EPC calculations, was developed by Kortus *et al.* [4] and Liu *et al.* [27]. The two band model based on Eliashberg equations was almost generally accepted and used by different authors. This model is a simplified model of the real four bands model, but it is a valid one, taking into account the similarities between the two $3D$ Fermi sheets and between the two $2D$ Fermi sheets. Based on them, when a strictly band calculation is not necessary, for the determination of T_c and for the gap functions, as in present study, there can be considered only a distinct gap for every $2D$, and respectively $3D$ sets of bands. Joas *et al.* [28] applied this model with a phonon spectral density $F(\Omega)$ having two peaks centered at $\omega_1 \cong 24meV$ for the π band and $\omega_2 \cong 67meV$ (the phononic E_{2g} mode) for the σ band, in order to explain tunneling experiments. In other studies [29,30], were deduced the temperature dependencies of the gap functions Δ_σ and Δ_π.

Here, we present a study of the two band Eliashberg model, for deducing self-consistently the gap and effective mass renormalization functions. The frequency response of these functions could offer useful information about the phononic coupling in appearance of the superconducting transition. This model is applied for deducing the temperature dependence of the two energy gaps in the superconducting state, revealing the superconducting transition and the value of the critical temperature, T_c.

There were two ways for the solving of Eliashberg equations. First of them was to solve the equations which contain dependencies of real frequency [31], and the second to solve this equations on the imaginary axis, summing on Matsubara frequencies [32]. In this case is needed an analytical continuation in order to obtain the dependencies on real frequency. In this paper is adopted the second way. We will start this analysis with the Eliashberg equations for a two band superconductor [29] which are similar in form with the case of a one band model. In this case will need four equations, two for the gaps and two for the renormalization functions, each corresponding to one of the two bands, σ and π:

$$Z_i(i\omega_n) = 1 + \frac{1}{\omega_n}\pi T \sum_{\nu_m} \sum_{j=\sigma,\pi} \left[\lambda_{ij}(i\omega_n - i\nu_m) - \mu_{ij}^*\right] \frac{\nu_m}{\sqrt{\nu_m^2 + \Delta_j^2(i\nu_m)}}$$

$$\Delta_i(i\omega_n) Z_i(i\omega_n) = \pi T \sum_{\nu_m} \sum_{j=\sigma,\pi} \left[\lambda_{ij}(i\omega_n - i\nu_m) - \mu_{ij}^*\right] \frac{\Delta_j(i\nu_m)}{\sqrt{\nu_m^2 + \Delta_j^2(i\nu_m)}} \quad (1)$$

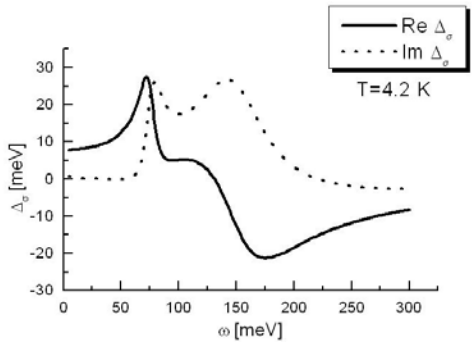
In Eq. (1) $\Delta_i(i\omega_n)$ are the superconducting order parameters of the σ ($i=\sigma$) and π ($i=\pi$) bands, $Z_i(i\omega_n)$ are the corresponding mass renormalization functions and μ_{ij}^* are the coulombian pseudopotentials. The sum is over the odd (fermionic) Matsubara frequencies $\nu_m = (m+1/2)\pi T$ and over the indexes $j=\sigma,\pi$ in order to include both intra and interband processes. The electron-phonon coupling (EPC) matrix element λ_{ij} is defined as:

$$\lambda_{ij}\left(i\omega_n - i\nu_m\right) = \int_0^{\infty} d\Omega \alpha_{ij}^2 F(\Omega) \frac{2\Omega}{\Omega^2 + \left(\omega_n - \nu_m\right)^2} \quad (2)$$

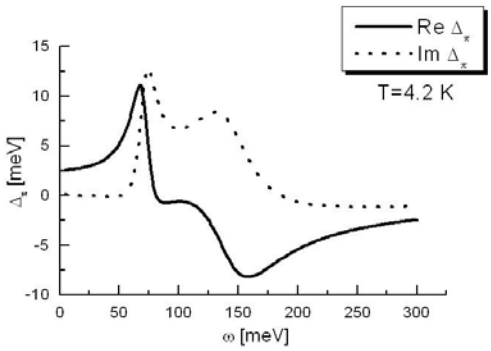
where $\alpha_{ij}^2 F(\Omega)$ are the Eliashberg spectral functions corresponding to each band. Considering the EPC as a matrix we assure to consider both intra and interband processes. For calculate these matrix elements the way of choosing the Eliashberg spectral functions is essential. C. P. Moca [29] analyzed a comparison between the temperature dependencies of the gaps in two different cases: the real Eliashberg spectral functions calculated in ref. [33] and a model function generated by a lorentzian dependence centered on the E_{2g} mode, but weighted for the each intra or inter band process with the appropriate factor, α_{ij}^2. Using the same α_{ij}^2 factors and the same values for the pseudopotentials μ_{ij}^* the results were similar. We use here this conclusion, working with a lorentzian model function weighted for intraband and interband interactions as described above, with a maximum at $64\ meV$ and a cut off interval of $30\ meV$ .The coulombian pseudopotential matrix elements, with values in agreement with that calculated in Ref. [34], were considered in a simple approximation, only for intraband processes: $\mu_{\sigma\sigma}^* = \mu_{\pi\pi}^* = 0.1$ and $\mu_{\sigma\pi}^* = \mu_{\pi\sigma}^* = 0$. The values for all parameters were chosen in order to obtain a good fit of experimental data in temperature dependencies of the gaps.

3. Results and discussions

As starting point, the two gaps were chosen $\Delta_\sigma = 7.5\,meV$ and $\Delta_\pi = 3.5\,meV$. With these values, at every temperature, in the Eqs. (1) were done summations over 1024 frequencies and the results were introduced again in equations, the process being stopped when the self-consistency of the gap functions was achieved. These solutions depending on imaginary frequency were numerically continued on real axis using Padé algorithm, and finally were obtained the dependencies on real frequency. The obtained dependencies at $T=4.2\ K$ are presented in Figs. 1. a and b.



a



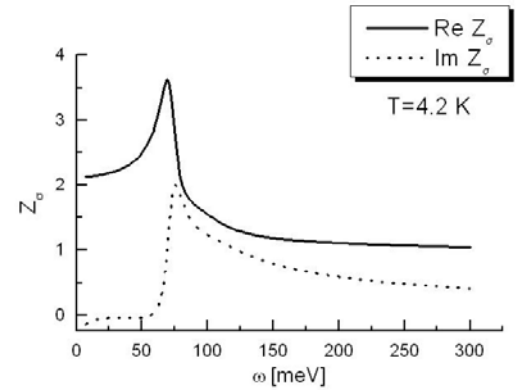
b

Fig. 1. Frequency dependence of the gap functions Δ_σ (a) and Δ_π (b) at the temperature $T=4.2\ K$. The values of parameters used for these graphs were chosen as explained in text: $\alpha_{\sigma\sigma} = 17.7$, $\alpha_{\pi\pi} = 6.5$, $\alpha_{\sigma\pi} = 1.0$, $\alpha_{\pi\sigma} = 2.0$ and the frequency of the phonons modes corresponding to the E_{2g} mode $\omega = 64\ meV$.

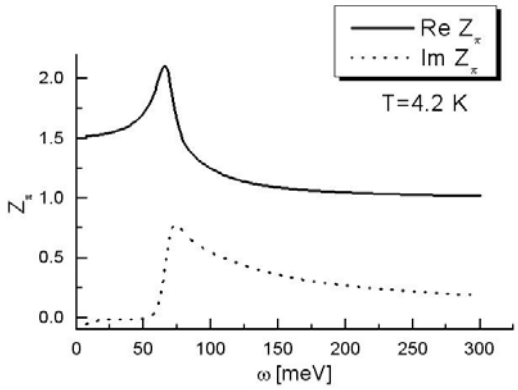
These curves are clearly connected with the electron – phonon coupling. As can be seen, the dependencies of $Re\,\Delta$ for the both two bands from Fig.1 present a maximum with a sharp slope at the chosen frequency $64\ meV$ (phononic E_{2g} mode). Above this frequency, the curves changes their sign due to the over screened pairing interaction. The imaginary part of the gap functions is an indicator of the phonon spectrum, starting to increase above the peak value of the E_{2g} mode, due to the process of phonons generation. In plus, the dependencies are very similar, Δ_σ being three times grater than Δ_π . This result confirms the assumption of weaker coupling by the phononic E_{2g} mode in π band, comparing with the σ band.

The interaction with the phonons modes is clearly seen, also, in frequency dependencies of the mass renormalization functions, presented in Fig. 2.

The frequency dependencies of the real and imaginary part of the mass renormalization function can be considered as an image of the EPC strength. For the both bands, is evident a peak around the value of the E_{2g} mode. These graphs lead to the same conclusion as those from Fig. 1, regarding the role of the in boron plane vibrations on pairing interaction of quasiparticles. The larger value of mass renormalization in σ band is illustrative for the larger coupling strength in this band. The result is in accordance with the larger value of the gap in σ band and suggests that the superconductivity mainly occur in this band, while in the π band it could be considered as induced from σ band via interband scattering.



a)



b)

Fig. 2. Frequency dependence of the mass renormalization functions Z_σ (a) and Z_π (b) at the temperature $T=4.2\,K$. The values of the parameters of the model were the same as for the gap dependencies represented in Fig. 1.

The validity of the model can be verified by direct comparison with experimental results. This comparison is possible for the temperature dependence of the gaps inside the two bands, being shown in Fig. 3. As can be seen, the theoretical calculated dependencies in our two band model fit very well the experimental measurements for the both gaps dependencies on temperature in superconducting state.

In above mentioned paper, Joas *et al.* [28] chose two peaks in phonon spectrum, each for each band: one of low energy ($\cong 24\,meV$) for the π band and other of high energy ($\cong 67\,meV - E_{2g}$ mode) for the σ band. They found similar shape of the curves, but notable differences between the graphs inside the σ and the π bands. They concluded that the superconductivity originates in both bands as an effect of the strong interactions with phonons described by the two modes. From our study, the very well fit of experimental data by the graphs from Fig. 3 can be considered a strong argument on the role of the phonons of E_{2g} mode in superconductivity of MgB_2.

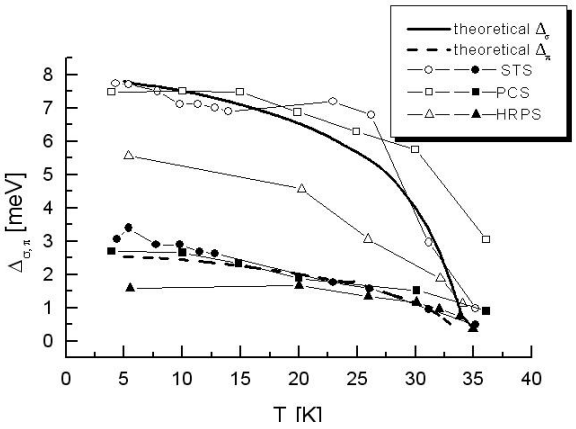


Fig. 3. Temperature dependence of the energy gaps for both the two bands. The experimental results, were subtracted from Refs. [3], [15], [18], [19].

A very useful result for the investigation of the electron-phonon coupling strength is the factor $2\Delta(0)/T_c$. From the results represented in Fig. 3, the obtained values for the gaps were: $\Delta_\sigma(0)=7.8\,meV$ and $\Delta_\pi(0)=2.5\,meV$. The critical temperatures were slightly different, being $T_c \cong 37K$ for σ band and $T_c \cong 36K$ for π band. The values differ from some experimental results, but are in good agreement with others [3, 31]. With these values, we found $2\Delta_\sigma(0)/T_c \cong 4.8$ and $2\Delta_\pi(0)/T_c \cong 1.7$. It is evident that the first value is much grater and the second much smaller than the weak coupling BCS-type value $2\Delta(0)/T_c = 3.5$. It can be considered an argument for the intermediate or even strong electron - phonon coupling scenario in explanation of the superconductivity in MgB_2.

4. Conclusions

In this paper, we report results obtained from numerical calculation performed inside a two band Eliashberg model. The model is based on the existence of the two different Fermi sheets: a quasi $2D$ cylindrical surface corresponding to the interaction of the p_x and p_y orbitals of B inside the boron layer, and a $3D$ tubular network corresponding to the interaction of the p_z orbitals of B. In explanation of the superconductivity in MgB_2, the obtained results confirm the correctness of the assumption that the electron-phonon coupling is mainly due to phonons of E_{2g} mode for both two bands. All frequency dependencies for the gap and mass renormalization functions reveal that the interaction in the π band should be considered more induced from interaction between electrons and high energy phonons

inside the σ band via interband scattering. The obtained ratio $2\Delta(0)/T_c$ in the two bands, in good agreement with experimental data, is higher in the σ band and lower in the π band than the weak coupling BCS -type value, suggesting that for MgB_2 is applicable the strong electron – phonon coupling approximation.

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