Localized states within the gap in a two-band superconductor

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We present results for strong-coupling calculations for the density of states in the presence of magnetic impurities in a two-band superconductor. Our calculations were done for the particular case of a MgB_2 compound where two bands (σ and π *B*-like) intersect the Fermi level. If only the π band is responsible for superconductivity, then an impurity band will form in the energy gap of the π band. If the σ band is involved, then new features may be found in the density of states at frequencies between the superconducting gaps corresponding to π and σ bands. The validity of our results can be directly verified by measuring the density of states in the presence of magnetic impurities using tunneling experiments in MgB_2. We also present analytical results for the doping dependence of the critical temperature.

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Since the discovery of superconductivity in MgB_2 by Nagamatsu *et al.*[1] with a critical temperature as high as $T_C = 39$ K, a tremendous amount of experimental and theoretical work has been initiated for giving a reasonable explanation of the superconducting properties of this compound. There is not yet a consensus whether the strong electron-phonon interaction[2] or the hole superconductivity[3] is responsible for superconductivity in MgB_2. Both scenarios seem to be in agreement with the large amount of experimental data[4–7] and in favor of *s-wave* superconductivity. Other experiments such as tunneling[8] and specific heat[9] have pointed out the presence of two gaps. The two-band superconductivity model was first proposed by Suhl *et al.*[10] in the framework of BCS theory as an academic problem. Later the model was applied to cuprate superconductors by Kresin *et al.* in the framework of Eliashberg theory.[11]

The aim of this paper is to conduct an experiment on MgB_2, whose qualitative outcome can, in principle, decide the number of the bands in MgB_2 involved in superconductivity. We consider the effect of paramagnetic impurities, treated within the Shiba approximation,[12] on the density of states in MgB_2. The first generalization of magnetic alloy theory to include strong-coupling effects within the Eliashberg theory was given by Schachinger[13] and further developed by others.[14] We generalize these results by considering the case of two-band superconductivity.[15] The Eliashberg equations for the two-band model were solved previously[16] in the case of clean superconductors and in the presence of nonmagnetic impurities for explaining the physical properties such as penetration depth and nuclear-spin relaxation in the superconducting state. In our calculations the numerical results for the quasiparticle density of states are obtained indirectly from the analytical continuation to the real frequency axis of the gap functions using a Padé approximation.[17] We have calculated the gap functions for a large number of Matsubara frequencies (we have used 2048 Matsubara frequencies) $i\omega_n$. When magnetic impurities are considered the perturbation potential is $V_I(\mathbf{r}-\mathbf{R}_I)=U(\mathbf{r}-\mathbf{R}_I)+J(\mathbf{r}-\mathbf{R}_I)\sigma\mathbf{S}$ where $\mathbf{R}_I$ is the impurity location. U describes the non-spin-flip interaction and the second term is the spin-flip interaction that is considered in the classical limit[19] ($S\to\infty$, $J\to 0$). $\mathbf{S}$ is the impurity spin which is a classical vector. The interaction term is treated based on a *T*-matrix approximation where multiple scattering on the magnetic impurity is considered, in contrast with Abrikosov-Gorgov theory[20] where only the Born approximation was taken into account. Although Shiba's theory applies to the case where higher partial wave electron-impurity scattering is included, the papers which have been based on the theory have all assumed lower scattering waves. In our approximation only the *s*-wave channel is considered. The derivation of the Eliashberg equations for the two-band model is similar to the case of one band.[13] When magnetic impurities are included the equations are

$$\Delta_\sigma(i\omega_n)=\frac{1}{Z_\sigma(i\omega_n)}\pi T\sum_{\omega_m}\left[(\lambda_{\sigma\sigma}(i\omega_n-i\omega_m)-\mu^\star_{\sigma\sigma})\times f_\sigma(i\omega_m)+\{\lambda_{\sigma\pi}(i\omega_n-i\omega_m)-\mu^\star_{\sigma\pi}\}f_\pi(i\omega_m)\right]+\frac{\Gamma^{(2)}_{\sigma\sigma}}{Z_\sigma(i\omega_n)}f_\sigma(i\omega_n)\frac{\omega_n^2+\Delta_\sigma^2(i\omega_n)}{\omega_n^2+\varepsilon_{\sigma\sigma}\Delta_\sigma^2(i\omega_n)}+\frac{\Gamma^{(2)}_{\sigma\pi}}{Z_\sigma(i\omega_n)}f_\pi(i\omega_n)\frac{\omega_n^2+\Delta_\pi^2(i\omega_n)}{\omega_n^2+\varepsilon_{\sigma\pi}\Delta_\pi^2(i\omega_n)},$$

$$\Delta_\pi(i\omega_n)=\frac{1}{Z_\pi(i\omega_n)}\pi T\sum_{\omega_m}\left[\{\lambda_{\pi\sigma}(i\omega_n-i\omega_m)-\mu^\star_{\pi\sigma}\}\times f_\sigma(i\omega_m)+\{\lambda_{\pi\pi}(i\omega_n-i\omega_m)-\mu^\star_{\pi\pi}\}f_\pi(i\omega_m)\right]+\frac{\Gamma^{(2)}_{\pi\sigma}}{Z_\pi(i\omega_n)}f_\sigma(i\omega_n)\frac{\omega_n^2+\Delta_\sigma^2(i\omega_n)}{\omega_n^2+\varepsilon_{\pi\sigma}\Delta_\sigma^2(i\omega_n)}+\frac{\Gamma^{(2)}_{\pi\pi}}{Z_\pi(i\omega_n)}f_\pi(i\omega_n)\frac{\omega_n^2+\Delta_\pi^2(i\omega_n)}{\omega_n^2+\varepsilon_{\pi\pi}\Delta_\pi^2(i\omega_n)},$$

$$Z_\sigma(i\omega_n)=1+\frac{1}{\omega_n}\pi T\sum_{\omega_m}[\lambda_{\sigma\sigma}(i\omega_n-i\omega_m)g_\sigma(i\omega_m)+\lambda_{\sigma\pi}(i\omega_n-i\omega_m)g_\pi(i\omega_m)]+\frac{\Gamma^{(1)}_{\sigma\sigma}}{Z_\sigma(i\omega_n)}g_\sigma(i\omega_n)\frac{\omega_m^2+\Delta_\sigma^2(i\omega_m)}{\omega_m^2+\varepsilon_{\sigma\sigma}\Delta_\sigma^2(i\omega_m)}+\frac{\Gamma^{(1)}_{\sigma\pi}}{Z_\sigma(i\omega_n)}g_\pi(i\omega_n)\frac{\omega_m^2+\Delta_\pi^2(i\omega_m)}{\omega_m^2+\varepsilon_{\sigma\pi}\Delta_\pi^2(i\omega_m)},$$

$$Z_\pi(i\omega_n)=1+\frac{1}{\omega_n}\pi T\sum_{\omega_m}[\lambda_{\pi\sigma}(i\omega_n-i\omega_m)g_\sigma(i\omega_m)+\lambda_{\pi\pi}(i\omega_n-i\omega_m)g_\pi(i\omega_m)]+\frac{\Gamma^{(1)}_{\pi\sigma}}{Z_\pi(i\omega_n)}f_\sigma(i\omega_n)\frac{\omega_n^2+\Delta_\sigma^2(i\omega_n)}{\omega_n^2+\varepsilon_{\pi\sigma}\Delta_\sigma^2(i\omega_n)}+\frac{\Gamma^{(1)}_{\pi\pi}}{Z_\pi(i\omega_n)}f_\pi(i\omega_n)\frac{\omega_n^2+\Delta_\pi^2(i\omega_n)}{\omega_n^2+\varepsilon_{\pi\pi}\Delta_\pi^2(i\omega_n)}, \quad (1)$$

where we have introduced the following notations for the functions g and f:

$$g_i(i\omega_n)=\frac{\omega_n}{\sqrt{\omega_n^2+\Delta_i^2(\omega_n)}},$$

$$f_i(i\omega_n)=\frac{\Delta_i(i\omega_n)}{\sqrt{\omega_n^2+\Delta_i^2(\omega_n)}}, \quad (2)$$

and

$$\lambda_{ij}(i\omega_n-i\omega_m)=\int_0^\infty d\omega\,\alpha^2_{ij}F(\omega)\frac{2\omega}{\omega^2+(\omega_n-\omega_m)^2}. \quad (3)$$

In Eqs. (1)–(3) $\Delta_i(i\omega_n)$ are the superconducting order parameters corresponding to the σ $(i=\sigma)$ and the π $(i=\pi)$ bands and $Z_i(i\omega_n)$ are the corresponding renormalization factors. The first term (sum over frequencies) in each equation is due to the intra- and interband phonon scattering while the last two terms are due to the impurity scattering in and between the bands. The parameters Γ_{ij} are defined as $2\Gamma^{(1)}_{ij}=1/\tau^{(1)}_{ij}+1/\tau^{(2)}_{ij}$ and $2\Gamma^{(2)}_{ij}=1/\tau^{(1)}_{ij}-1/\tau^{(2)}_{ij}$ where $\tau^{(1)}_{ij}$ is the non-spin-flip scattering lifetime and $\tau^{(2)}_{ij}$ is the spin-flip scattering lifetime of the magnetic impurity. Γ_{ij} is proportional with the impurity concentration n_i. ε_{ij} are related with the scattering phase in the *s-wave* channel[13] $\varepsilon_{ij}=\cos(\delta^+-\delta^-)$, where $\tan(\delta^\pm)=U\pm JS$. In our calculations we consider that scattering between bands is not important so the scattering rates $\tau^{-1}_{\pi\sigma}$ and $\tau^{-1}_{\sigma\pi}$ can be neglected. In order to motivate our approximation we consider first the case of the single impurity model. In this case the p_x,p_y orbitals of the σ band and the p_z orbitals of the π band may hybridize with the same impurity orbital. This hybridization will lead to a finite interband scattering between bands.[18] The only qualitative feature observed when increasing the interband scattering was a broadening of the bound states corresponding to the σ band (transformation into a resonance with a finite width) while their position remained fixed. The bound states corresponding to the π band remain practically unchanged with modifying the interband scattering. When a finite concentration is considered the resonances corresponding to each band transform into a impurity band.[12] A large scattering between bands may lead to a broadening of the observed features in the density of states of each band. However if the magnetic impurities are randomly distributed in the material the corresponding σ- and π-band orbitals couple with different orbitals of the magnetic impurities so the charge transfer between the bands is very small. In our study we considered this a good approximation, we neglected the scattering between bands mediated by the magnetic impurities, and considered that what was responsible for interband electron interaction are phonons only. In the case of the two-band model there are four Eliashberg functions $\alpha^2_{ij}F(\omega)$ instead of only one, as in the case of the single-band model. Their frequency dependence was recently calculated in Ref. 22 and it was found that all present a sharp peak at a frequency corresponding to the E_{2g} phononic mode. In our calculations we will use a Lorentzian form for the phonon density of states, which was demonstrated[16] to model the experimental data for the temperature dependence of the gap functions. The Lorentzian is centered at a frequency corresponding to the E_{2g} mode ($E_{2g}=67$ meV). For each band we keep the same $F(\omega)$ constant and vary only the weighting factors α_{ij} in order that the temperature dependence of the calculated gaps fit the experimental data. The critical temperature can be defined as the highest temperature below which there are nonvanishing solutions for the gap functions $\Delta_i(i\omega_n)$. Including magnetic impurity terms in Eliashberg equations has a drastic effect on the frequency dependence of the gap functions $\Delta(i\omega_n)$ and of the renormalization functions $Z(i\omega_n)$. In Fig. 1 we represent the frequency dependence of the gap functions and the renormalization constants for the σ band. Similar results are obtained also for the π band (see also Ref. 16). The real parts of the gap functions start to decrease as we increase the scattering rates and the imaginary parts become negative below the leading edge gap [given by the equation $\mathrm{Re}\{\Delta(\omega=\Delta_0)\}=\Delta_0$]. In the clean limit below the leading edge gap the imaginary part of the gap functions vanishes. The most important difference between alloys and the pure limit is the low-frequency behavior of the imaginary part of the renormalization constant $Z_i(i\omega_n)$ which acquires a $1/\omega$ dependence due to the impurity scattering term. We performed numerical calculations for a large spectrum of magnetic impurity lifetimes and we found qualitatively similar results for the frequency dependence of the gap functions and for the renormalization functions $Z_i(\omega)$. Anisotropy of the band structure may lead to modification of the gap function for frequencies larger than the leading edge gap energy, therefore, we did not take into account the full **k** dependence of the gap and of the renormalization function. We consider an isotropic single-particle excitation for the two Fermi-surface sheets, which is a reasonable approximation[21] for the present problem. In Fig. 1 we present the result for the clean limit together with the case when $1/\tau^{(1)}_{\sigma\sigma}=3.0$, $1/\tau^{(2)}_{\sigma\sigma}=1.5$, $1/\tau^{(1)}_{\pi\pi}=2.0$, $1/\tau^{(2)}_{\pi\pi}=1.0$, and $\varepsilon_{ij}=0.85$. All the other scatter-

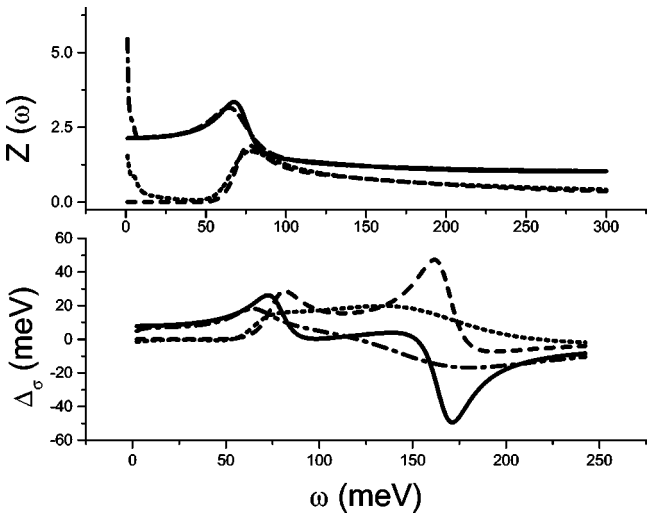

FIG. 1. Frequency dependence of the real part (solid line) and the imaginary part (dashed line) of the gap functions, and real part (solid line) and imaginary part (dashed line) of the renormalization function for the σ band in the clean limit. The same quantities are presented in the presence of impurities. Real part of gap function (dash-dotted line), and imaginary part of the gap function (short dotted line), real part of the renormalization constant (dash-dotted line), and imaginary part of the renormalization function (short dotted line). The values of the scattering rates are in this case $1/\tau_{\sigma\sigma}^{(1)}=3.0$, $1/\tau_{\sigma\sigma}^{(2)}=1.5$, $1/\tau_{\pi\pi}^{(1)}=2.0$, $1/\tau_{\pi\pi}^{(2)}=1.0$, and $\varepsilon_{ij}=0.85$. All the other scattering rates were considered to be zero.

ing rates were considered to be zero. The scattering rate between the bands has no other qualitative effect except that the leading edge gaps corresponding to each band start to converge to the same value. All these modifications in the frequency dependence of the gap functions and of the renormalization constants lead to the formation of an ''impurity band,'' within the density of states, that grows to fill the gap at a finite concentration of magnetic impurities. This effect is observed for each band separately. For the completeness of our work we present also analytical results for temperature dependence of the gap functions near the critical temperature, near $T=0$ K, and for the doping dependence of the critical temperature. We have studied the influence of the magnetic impurities on the critical temperature T_C. The system (1) is not tractable analytically but a numerical solution is possible. In any case, considering the weak-coupling limit, it is possible to transform the Eliashberg equations into BCS equations for a two-band model for which the solution for the critical temperature is known.[10] The weak-coupling limit is characterized by the following approximations:

$$\lambda_{ij}(i\omega_n - i\omega_m)=\begin{cases}\lambda_{ij} & |\omega_n|,|\omega_m|<\omega_C,\\ 0 & \text{otherwise},\end{cases} \tag{4}$$

and for the gap functions,

$$\Delta_i(i\omega_n,T)=\begin{cases}\Delta_i(T) & |\omega_n|<\omega_C,\\ 0 & |\omega_n|>\omega_C,\end{cases} \tag{5}$$

where ω_C is the frequency cutoff which is of the order of the Debye energy and for the case of MgB_2 can be considered to be 100 meV ($\Theta_D\simeq 750\div 880$ K).[23] Within these approximations the renormalization functions become $Z_\sigma(i\omega_n)=1+\lambda_{\sigma\sigma}+\lambda_{\sigma\pi}$, and $Z_\pi(i\omega_n)=1+\lambda_{\pi\pi}+\lambda_{\pi\sigma}$. By introducing the notations $V_{ij}=(\lambda_{ij}-\mu_{ij}^{\star})/(1+\lambda_{i\sigma}+\lambda_{i\pi})$, it is possible to simplify the analytical solution of the gap equations. In particular we have reobtained the gap equations first derived by Suhl *et al.* and the critical temperature expression.[10] We have also calculated the ratio $2\Delta_i/T_C$ which was found to be $2\Delta_i/T_C=2e^{-\gamma}\pi e^{B_i}$ where

$$B_i=1+\frac{V_{ii}V_{jj}-V_{ij}V_{ji}+2(V_{ii}-V_{jj})+4V_{ij}}{2\sqrt{(V_{ii}-V_{jj})^2+4V_{ij}V_{ji}}}. \tag{6}$$

An interesting result emerges from these calculations regarding the value of $2\Delta_i/T_C$ which was found to be nonuniversal in contrast with the BCS theory where this value is universal and equal to $2\Delta_i/T_C=3.52$. In the case when the impurities are considered we have an extra term for the renormalization constant Z_i due to the scattering on the impurities. In this case we reobtained the results of Ref. 24, which were written here for completeness:

$$\ln\frac{T_C}{T_{C0}}=f_+ +\frac{\sqrt{A}-\sqrt{A_0}}{2(V_{\sigma\sigma}V_{\pi\pi}-V_{\sigma\pi}V_{\pi\sigma})}, \tag{7}$$

where $A=(V_{\sigma\sigma}+V_{\pi\pi})^2+4[f_-^2(V_{\sigma\sigma}V_{\pi\pi}-V_{\sigma\pi}V_{\pi\sigma})+f_-(V_{\sigma\sigma}-V_{\pi\pi})-1](V_{\sigma\sigma}V_{\pi\pi}-V_{\sigma\pi}V_{\pi\sigma})$, and $A_0=(V_{\sigma\sigma}-V_{\pi\pi})^2+4V_{\sigma\pi}V_{\pi\sigma}$. The coefficients $f_\pm$ are given by the following relations: $f_+=1/2[\Psi(1/2+\rho_\sigma)+\Psi(1/2+\rho_\pi)]-\Psi(1/2)$, and $f_-=1/2[\Psi(1/2+\rho_\sigma)-\Psi(1/2+\rho_\pi)]$. In the last two equations $\rho_i=(\Gamma_{i\sigma}^{(1)}+\Gamma_{i\pi}^{(1)})/2\pi T$. Solving Eq. (7) it is found that the critical temperature starts to decrease as we increase the doping, and at a critical doping the critical temperature goes to zero. The analytical results of Eqs. (6) and (7) were obtained in the weak-coupling theory and should be considered qualitatively for comparison with similar results for the one-band model[24] where only one interaction term exists in contrast with four interaction terms considered in the two-band model.

The quasiparticle density of states can be measured directly by tunneling experiments. It is related only to the gap functions and can be calculated directly from the solutions of Eliashberg equations:

$$N_S^{(i)}(\omega)=\mathrm{Re}\left[\frac{\omega}{\sqrt{\omega^2-\Delta^2(\omega)}}\right]. \tag{8}$$

This result is valid for the case of the clean limit and for the case of alloys also. In Fig. 2 we have represented the calculated frequency dependence of the density of states in the presence of magnetic impurities. The main figure presents the density of states for each band. The Shiba bound states, which correspond to the case of a single impurity,[18] transform into impurity bands which start to grow with increasing doping. At the same time the critical temperature decreases. The qualitative behavior presented in Fig. 2 occurs for a large range of scattering rates and for different values of the impurity parameter ε_{ij}. The left inset shows the total density of states calculated as a weighted sum with a 10% contribution from the σ band and a 90% contribution from the π band. If both bands give a contribution to the measured density of states a bias dependence conductance is expected in a

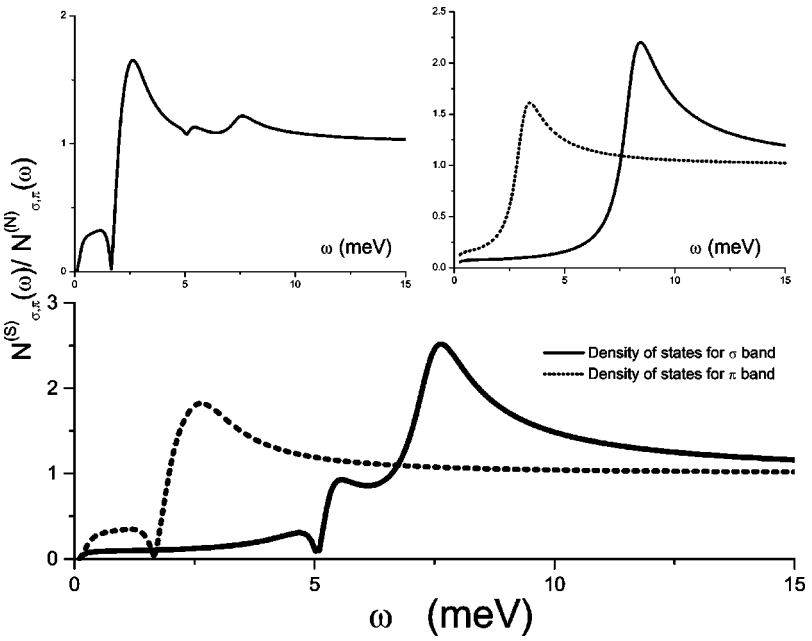

FIG. 2. Density of states for σ and π bands in the presence of the magnetic impurities. The right inset shows the density of states in the clean limit. The left inset represents the total density of states as a weighted average of the densities of each band. The values for the scattering rates are similar to those in Fig. 1.

tunneling experiment in the presence of magnetic impurities. This may help find which band gives a contribution to the total density of states in the presence of magnetic impurities so it is possible to find the number of bands which are responsible for the superconductivity in MgB_2. If the small feature at the energy between the gaps presented in the left inset of Fig. 2 is not observed, two possibilities may provide an explanation. The first is that the σ band gives no contribution to the total density of states and the second is that the σ- and π-band orbitals hybridize with the same impurity orbital, which in the case of random impurities is improbable. These features calculated theoretically in the density of states we believe can be observed experimentally in tunneling experiments when doping MgB_2 with a finite concentration of magnetic impurity.

In conclusion we have studied the influence of magnetic impurity on the density of states of a two-band superconductor. We have found that there is a measurable effect on both densities of states corresponding to the σ and π bands for frequencies below the gap energy corresponding to each band. In break junction tunneling experiments of Ref. 6 only the π band gives a contribution to the tunneling current due to its three-dimensional nature while the other band, due to its quasi-two-dimensional nature, does not contribute to the tunneling current. The effect that we observed in density of states can be experimentally measured by magnetically doping MgB_2. Using break junctions techniques the bulk properties of the system can be investigated in this limit. We think that the predominant contribution to the tunneling current will be from π band while the σ will contribute less due to its 2D nature. Using scanning-tunneling microscopy it is also possible to measure the density of states in the presence of magnetic impurities and check the validity of our theory.

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