Effects of paramagnetic impurities on two-band superconductor

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I calculated the effect of magnetic impurities on the normal and superconductive properties of a multiband s-wave superconductor by direct solution of the two-band Eliashberg equations. In this way I determined the critical temperature, the values of the superconductive gaps, the shape of the superconductive density of states and other physical quantities that depend on the concentration of magnetic impurities. I found that the gaps and the penetration lengths display an unusual behaviour as a function of temperature. I examine the possibility that the presence of a negative induced gap raises the critical temperature.

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A specific, but representative case of anisotropic superconductivity is multiband superconductivity where the order parameter is different in different bands. The more famous and clear case is the magnesium diboride \[1\] where the two gaps are observed in several experiments. Some properties of this material changes markedly from the more famous and clear case is the magnesium diboride \[1\].

Let us start from the generalization of the Eliashberg theory \[6\] for systems with two bands \[7, 8\] , that has already be used with success to study the MgB2 system \[4, 5\]. By Mn \[4, 5\].

Some properties of this material changes markedly from the more famous and clear case is the magnesium diboride \[1\].

The solution of the Eliashberg equations requires as input: i) the four (but only three independent \[7\]) electron-phonon spectral functions \[\alpha^2_\sigma(\omega)F(\omega)\]; ii) the four (but only three independent \[7\]) elements of the Coulomb pseudopotential matrix \[\mu^*(\omega_c)\]; iii) the two (but only one effective \[7\]) non-magnetic impurity scattering rates \[\Gamma^N_{ij}\]; iv) the four (but only three independent \[7\]) paramagnetic impurity scattering rates \[\Gamma^M_{ij}\]. The four spectral functions \[\alpha^2_\sigma(\omega)F(\omega)\] , that were calculated for pure MgB2 in ref. \[11\], have the following electron-phonon coupling constant: \[\lambda_{\sigma\sigma}(x=0)=1.017, \lambda_{\pi\pi}(x=0)=0.448, \lambda_{\sigma\pi}(x=0)=0.213\] and \[\lambda_{\pi\sigma}(x=0)=0.156\].

As far as the Coulomb pseudopotential is concerned, I use the expression calculated for pure MgB2 \[13\]:

\[
\mu^* = \begin{bmatrix}
\mu^*_{\sigma\sigma} & \mu^*_{\sigma\pi} \\
\mu^*_{\pi\sigma} & \mu^*_{\pi\pi}
\end{bmatrix} = \begin{bmatrix}
\mu^*_{\sigma\sigma} & \mu^*_{\sigma\pi} \\
\mu^*_{\pi\sigma} & \mu^*_{\pi\pi}
\end{bmatrix} = \begin{bmatrix}
\frac{2.23}{N^N_{\sigma\sigma}(E_F)} & \frac{1}{N^N_{\sigma\pi}(E_F)} \\
\frac{1}{N^N_{\pi\sigma}(E_F)} & \frac{2.48}{N^N_{\pi\pi}(E_F)}
\end{bmatrix}
\]

(3)

where \[\mu(\omega_c, x)\] is a free parameter and \[N^N_{\sigma\sigma}(E_F, x)\] is the total normal density of states at the Fermi level. For obtaining the experimental critical temperature of pure MgB2 case \((T_c = 39.4 \text{ K})\) we fix \[\mu(\omega_c) = 0.03105\] with cut-off energy \[\omega_c = 500 \text{ meV}\] and maximum energy \[570 \text{ meV}\]. In all our calculations I use \[11\] \[N^N_{\sigma\sigma}(E_F) = 0.30\] states/(cell eV) and \[N^N_{\pi\pi}(E_F) = 0.41\] states/(cell eV). In this work I study only the effect of paramagnetic impurities so is always \[\Gamma^N_{ij} = 0\]. In fig. 1 we can see the effect of magnetic impurities on the critical temperature in four limit cases. The stronger reduction of \[T_c\] is when the \[\Gamma^M_{\sigma\sigma}\] is preponderant while the effect of the \[\Gamma^M_{\pi\pi}\] is weak. A part the \[\Gamma^M_{\pi\pi}\] cases a small amount of impurities is safe for reduce \[T_c\] in a considerable way.
the fact of thinking the MgB$_2$ doped with paramagnetic impurities as a system perturbed and not as new material with different electron-phonon coupling constant, phonon energies and Coulomb pseudopotentials. In fig. 2 we can see the calculated penetration depth by solution of imaginary axis Eliashberg equations \[14\]. The curve are remarkably different of pure case especially when is of imaginary axis Eliashberg equations \[14\]. The curve is impossible to determine the sign of $\Delta$.

In fig. 3 panel a we can see the calculated values of $\Delta_i(i\omega_n=0)$ as function of the temperature always with $T_c = 28K$. When are present magnetic impurities in the interband channel the curve has a maximum more evident if the impurity content is bigger. In the $\Gamma^\sigma_{\omega\pi} \neq 0$ case the $\Delta_\pi(i\omega_n=0)$ gap is negative in a small range of temperature (experimentally it is found that the presence of magnetic interband scattering is very small \[4\]). In the panel b we can see the calculated tunneling conductance at $T = 4K$: in this case the curves are similar for the effect of smearing of the temperature: it is necessary to go to lower temperatures for noting appreciable differences. Of course from experiments of quasiparticle tunneling it is impossible to determine the sign of $\Delta_\sigma$. In the fig. 4 it is possible see the calculated values of $\Delta_c(i\omega_n=0)$ as function of the temperature with $T_c = 18K$ (panel a) and $T_c = 13.3K$ (panel b). In the panel b we can note that, in the $\Gamma^\pi_{\sigma\pi} \neq 0$ case, there is a range of temperatures where $\Delta_\pi(i\omega_n=0) > \Delta_\sigma(i\omega_n=0)$.

It is important remember that in presence of strong coupling electron-phonon interaction or magnetic impurities the value of $\Delta_c(i\omega_n=0)$ obtained by solving the imaginary axis Eliashberg equations and the $\Delta_\sigma$ obtained by real axis formulation can be very different so it is necessary always or the analytical continuation \[13\] or the real axis solution for determine the physical quantities comparable to measurable experimental gaps.

If we put the interband electron phonon coupling constant $\lambda_{\pi\pi}$ (of course also $\lambda_{\pi\sigma}$) and Coulomb pseudopotential matrix $\mu_{ij}$ equal to zero, in the MgB$_2$ case, I find an hypothetic material with $T_c = 45.55K$ and only a superconductive gap in the $\sigma$ band because the $\pi$ band is superconductive only for the presence of interband term. In the MgB$_2$ case, the presence of interband term reduces $T_c$. If I calculate the critical temperature in function of $\lambda_{ij}$ with all other parameters equal to MgB$_2$ case, I found that when $\lambda_{\pi\pi} = \lambda_{\pi\pi}^{MgB_2}$ the $T_c$ is next to a minimum as we can see in fig. 5.

Now, if is only $\lambda_{ij} = 0$, $i \neq j$ but the matrix $\mu_{ij}$ has the usual MgB$_2$ values it can induce a negative gap in the $\pi$ band and overall raise the critical temperature until 48.75K. We can think of obtaining a negative $\Delta_c(i\omega_n=0)$ gap i.e., roughly, when applies the condition $\lambda_{ij} - \mu_{ij}^* < 0$, $i \neq j$, with chemical or field effect doping where x is the doping content. I assume, for simplicity, $\lambda_{\pi\sigma}(x) = \lambda_{\pi\sigma}(0)N_N^\pi(E_F, x)/N_N^\pi(E_F, 0)$ and $\mu_{\pi\sigma}(x) = \mu_{\pi\sigma}(0)N_N^{\pi\pi}(E_F, x) \cdot N_N^{\pi\pi}(E_F, 0)/N_N^{\pi\pi}(E_F, x)$ so I find, in the MgB$_2$ case, $N_N^\pi(E_F, x) <$
other way for having a negative gap is if roughly so it is necessary to study in depth the problem. An order parameter (eq. 2) and a negative gap in the channel the two cases is in the structure of Eliashberg equations: phononic components but with the interband Coulomb the interband coupling is negative for example without case, decreases: i.e. it is possible to have an induced neg-

glect the presence of disorder, i.e. I put $\Gamma_{\pi\pi}^M = 0$ (dotted line); panel b: the calculated tunneling conductance, at $T = 4K$, in the three different magnetic doping case: $\Gamma_{\sigma\pi}^M \neq 0$ (solid line), $\Gamma_{\sigma\pi}^M = \Gamma_{\pi\pi}^M \neq 0$ (dashed line), $\Gamma_{\pi\pi}^M \neq 0$ (dotted line).

For example in the case of Al doping, where, of course, I neglect the presence of disorder, i.e. I put $\Gamma_{\pi\pi}^M = 0$, this condition is safe only for $x > 0.46$ when the material isn’t more a superconductor! To raise the critical temperature is more difficult because $T_c$ decreases primarily if $\lambda_{\sigma\sigma}$ lowers and, in our rough model, $\lambda_{\sigma\sigma}(x) = \lambda_{\sigma\sigma}(0)N_N^\sigma(E_F, x)/N_N^\sigma(E_F, 0)$ decreases with $N_N^\sigma(E_F, x)$ so it is necessary to study in depth the problem. An other way for having a negative gap is if roughly $\lambda_{ij} - \mu_j - \Gamma_{ij}^M < 0$, $i \neq j$, but the critical temperature, in this case, decreases: i.e. it is possible to have an induced negative gap or with interband magnetic impurities or whenalue when the interband coupling is negative for example without phononic components but with the interband Coulomb pseudopotential different from zero. The difference in the two cases is in the structure of Eliashberg equations: the Coulomb term is present only in the equation of the order parameter (eq. 2) and a negative gap in the channel.

$0.0311N_N^\sigma(E_F, x)/(0.3805N_N^\sigma(E_F, x) - 0.0311)$. For example in the case of Al doping, where, of course, I neglect the presence of disorder, i.e. I put $\Gamma_{\pi\pi}^M = 0$, this condition is safe only for $x > 0.46$ when the material isn’t more a superconductor! To raise the critical temperature is more difficult because $T_c$ decreases primarily if $\lambda_{\sigma\sigma}$ lowers and, in our rough model, $\lambda_{\sigma\sigma}(x) = \lambda_{\sigma\sigma}(0)N_N^\sigma(E_F, x)/N_N^\sigma(E_F, 0)$ decreases with $N_N^\sigma(E_F, x)$ so it is necessary to study in depth the problem. An other way for having a negative gap is if roughly $\lambda_{ij} - \mu_j - \Gamma_{ij}^M < 0$, $i \neq j$, but the critical temperature, in this case, decreases: i.e. it is possible to have an induced negative gap or with interband magnetic impurities or when the interband coupling is negative for example without phononic components but with the interband Coulomb pseudopotential different from zero. The difference in the two cases is in the structure of Eliashberg equations: the Coulomb term is present only in the equation of the order parameter (eq. 2) and a negative gap in the channel.
\(\pi\) produces a positive contribute in the more important channel \(\sigma\) so the critical temperature raises while in the case of interband impurities in the equation of the order parameter there is a positive contribute of the Coulomb term but a negative contribute of the impurity term and also, in the equation of renormalization function (eq. 1), a positive contribute of the impurity term that raises the value of the renormalization function but, for consequence, lowers the critical temperature.

I want remember that the possibility of a negative induced gap in a multiband system have been already previewed by A.A. Golubov et al. more ten years ago (see ref. 8).

In conclusion the effects of magnetic impurities can produce, in multiband superconductors, unusual behaviour as the temperature dependence of the order parameter and penetration depth but overall can induce superconductivity with negative order parameter in the eventual normal band.

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