Impurity suppression of the critical temperature in the iron-based superconductors

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We study the impurity suppression of the critical temperature $T_c$ of the FeAs superconductors theoretically based on the the $\pm s$-wave pairing state of a two band model. The effects of non-magnetic and magnetic impurities are studied with the $\tau$-matrix approximation, which can continuously treat impurity scattering from weak to strong coupling limit. We found that both magnetic and non-magnetic impurities suppress $T_c$ with a rate that is practically indistinguishable from the standard $d$-wave case despite a possibly large difference of the positive and negative $s$-wave order parameter (OP) magnitudes. This is because the density of states enters together with the OP magnitude for the scattering process.

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Introduction – The alluring prospect of opening a key window to understanding the mechanism of high temperature superconductivity (SC) has attracted fierce research activities in the iron based pnictides [1,2]. The first step towards this goal is to establish the pairing symmetry of the FeAs superconductors. Many ideas have been put forward to understand the seemingly conflicting experimental observations on the FeAs materials with regard to the pairing symmetry. Among them, particularly appealing is the sign reversing pairing state proposed by Mazin and coworkers [3]. It is the ground state of a two band superconductivity where both pairing order parameters on the two bands have full gaps while acquiring the $\pi$ phase shift between them, which is referred to as the $\pm s$-wave pairing state [4]. It was noticed early on that there is this type of solution to a multi-band BCS gap equation [5,6], and it is quite exciting that it seems to be actually realized in the pnictide superconductors. A repulsive interband interaction is turned to induce pairing by generating the sign reversal between the two pairing order parameters. The $\pm s$-wave state seems to be able to explain most of the experimental observations indicating the full gap behavior [7] as well as a gapless behavior [8,9,10].

In this paper, we wish to show that the relative phase of $\pi$ shows up in the impurity suppression of the critical temperature $T_c$, in an interesting way. We employ the $\tau$-matrix approximation in the weak coupling two band BCS theory. In the previous paper, using the same theoretical method, we reported that the impurity effects on the $\pm s$-wave state can introduce an unusual behavior in NMR $1/T_1$ relaxation rate [9]. Therefore, it would be interesting to study the effect of impurity on the $T_c$ suppression in this unconventional pairing state. The $T_c$ suppression by non-magnetic impurity is, as might be expected from the sign changing gap nature of the $\pm s$-wave state, in between the $s$-wave and $d$-wave pairing states. Unexpected, however, is that it is indistinguishably close to the standard $d$-wave case despite a large difference of the positive and negative OP magnitudes. We also found that magnetic impurities are more efficient pair breakers than non-magnetic impurities in the $\pm s$-wave pairing state and therefore magnetic impurities yield a faster $T_c$ suppression rate in the $\pm s$-wave pairing state than in the $d$-wave pairing state although it is a marginal difference with realistic parameters.

Formalism – We study a two band model for the FeAs superconductors (SC). The details were presented in the reference [11]. Assuming two SC order parameters, $\Delta_h$ and $\Delta_e$, on each band, the two coupled gap equations are written as

$$\Delta_h(k) = -\sum_{k'} [V_{hh}(k,k')\chi_h(k') + V_{he}(k,k')\chi_e(k')]$$

$$\Delta_e(k) = -\sum_{k'} [V_{eh}(k,k')\chi_h(k') + V_{ee}(k,k')\chi_e(k')]$$

(1)

where $V_{he}(k,k')$ is the phenomenological pairing interaction originating from the antiferromagnetic (AFM) correlation. The above gap equation permits two solutions. When the inter-band pairing interaction $V_{he}$ = $V_{eh}$ are repulsive and dominant over the intra-band interactions, the state where $\Delta_h$ and $\Delta_e$ have the relative phase of $\pi$, referred to as $\pm s$-wave pairing state, is the ground state. The pair susceptibility is given by

$$\chi_{h,e}(k) = \frac{T}{N(0)_{h,e}} \int_{-\omega_{AFM}}^{\omega_{AFM}} d\epsilon \frac{\tilde{\Delta}_{h,e}(k)}{\epsilon^2 + \tilde{\Delta}_{h,e}^2(k)}$$

(2)

where $N(0)_{h,e}$ are the DOS of the hole and electron bands, respectively, and $\omega_{AFM}$ is the cutoff energy of the pairing potential $V(q)$.

The impurity effects are included within the $\tau$-matrix ap-
proximation as
\[
\tilde{\omega}_n = \omega_n + \Sigma_{h,e}^0(\omega_n),
\tilde{\Delta}_{h,e} = \Delta_{h,e} + \Sigma_{h,e}^\perp(\omega_n),
\Sigma_{h,e}^\perp(\omega_n) = \Gamma \cdot T_{h,e}^{0.1}(\omega_n), \quad \Gamma = \frac{n_{imp}}{\pi N_{tot}},
\]
where \(\omega_n = T \pi (2n + 1)\) is the Matsubara frequency, \(n_{imp}\) the impurity concentration, and \(N_{tot} = N_h(0) + N_e(0)\) is the total DOS. The \(\tau\)-matrices \(\tau_{h,e}^{0.1}\) are the Pauli matrices \(\sigma_{h,e}\) components in the Nambu space. The impurity induced self-energies are calculated with the \(\tau\)-matrix generalized to a two band superconductivity as [9],
\[
\tau_{h,e}^{0.1}(\omega_n) = \frac{G_{h,e}^{0}(\omega_n)}{D} \quad (i = 0, 1; \ a = h, e),
\]
\[
D = c^2 + |G_{h}^{0}|^2 + |G_{e}^{0}|^2, \quad G_{h,e}^{0}(\omega_n) = \frac{N_{h,e}}{N_{tot}} \left( \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_{h,e}^2(k)}} \right),
\]
where \(c = \cot \delta_0\) is a convenient measure of scattering strength, with \(c = 0\) for the unitary limit and \(c > 1\) for the Born limit scattering. \(<\ldots>\) denotes the Fermi surface average.

Because we are interested in determining \(T_c\), we take \(T \to T_c\) limit and linearize the gap equation with respect to the order parameters. We obtain
\[
\tilde{\omega}_n = \omega_n(1 + \eta_0), \quad \tilde{\Delta}_{h,e} = \Delta_{h,e}(1 + \delta_{h,e}),
\]
where
\[
\eta_0 = \frac{\Gamma}{1 + c^2 |\omega_n|}, \quad \delta_{h,e} = \frac{\Gamma}{1 + c^2 |\omega_n|} \left( \frac{N_h \Delta_h + N_e \Delta_e}{\Delta_{h,e}} \right),
\]
with \(\tilde{N}_0 = N_{tot}/N_{tot}\). The pair susceptibility can be written as
\[
\chi_{h,e}(k) = \pi T \sum_n N(0)_{h,e} \frac{\delta_{h,e}(k)(1 + \delta_{h,e})}{|\omega_n(1 + \eta_0)|}.
\]
It is immediately clear that \(\eta_0 = \delta_0\) for a single band \(s\)-wave gap state and there is no renormalization of the pair susceptibility \(\chi_{h}(k)\) with the impurity scattering. This is just the Anderson theorem of \(T_c\) for the \(s\)-wave SC. In our two band case, it is more complicated to draw any simple conclusion. In particular, the signs of \(\delta_0\) and \(\delta_{h,e}\) are opposite because of the opposite signs of \(\Delta_{h,e}\).

Before we show the numerical results we can analyze a simpler case. The main pairing process in the \(\pm s\)-wave pairing state is the inter-band interaction so that we keep only \(V_{he} = V_{eh}\) interactions in the gap Eqs. (1) and (2), and use Eq. (12) to obtain
\[
\Delta_h = \pi^2 T^2 \sum_n \sum_m \lambda_{eff}^2 \frac{(1 + \delta_h)(1 + \delta_{h})}{|\omega_n(1 + \eta_0)|(|\omega_n(1 + \eta_0)|)} \Delta_h, \quad (13)
\]
where \(\lambda_{eff} = \sqrt{N_h N_e V_{he} V_{eh}}\) is the effective dimensionless coupling constant. This equation can be compared with the similarly reduced gap equation without impurities as
\[
\Delta_h = \pi^2 T^2 \sum_n \sum_m \lambda_{eff}^2 \frac{1}{|\omega_n(1 + \eta_0)|(|\omega_n(1 + \eta_0)|)} \Delta_h, \quad (14)
\]
which yields the standard single band \(s\)-wave result with \(T_0^0 \approx 1.14 \omega_{0} \exp(-1/\lambda_{eff})\). Eq. (13) would yield definitely smaller \(T_c\) than \(T_0^0\) because \(\delta_0\) is smaller in magnitude than \(\eta_0\). When both \(\delta_0\) are set to zero we obtain another reduced gap equation as
\[
\Delta_h = \pi^2 T^2 \sum_n \sum_m \lambda_{eff}^2 \frac{1}{|\omega_n(1 + \eta_0)|} \Delta_h, \quad (15)
\]
which is just the case that we would obtain for a double \(d\)-wave pairing state [11] where the anomalous self-energy corrections (\(\tilde{\delta}_0\)) are absent because of the sign-changing OP with equal sizes. Our case of Eq. (13) is not straightforward. If both \(\delta_0\) are positive (their magnitudes are always smaller than \(\eta_0\)), the \(T_c\) reduction would be simply in between the case of a \(s\)-wave (no suppression) and the case of a \(d\)-wave. But in the \(\pm s\)-wave case \(\tilde{\delta}_0\) will have always opposite signs and as a result the \(T_c\) reduction can be faster or slower than the \(d\)-wave case of Eq.(15). A simple rule is the following: in the leading approximation the reduction rate depends on the sign of the quantity \((\delta_0 + \delta_{h,e})\). If it is positive, the \(T_c\) reduction is slower than the \(d\)-wave case, and if it is negative, the \(T_c\) reduction is faster than the \(d\)-wave case.

We can utilize the relation \(|\Delta_h|/|\Delta_s| = \sqrt{N_e/N_h}\) as \(T \to T_c\) found in the minimal two band model in Ref.[11], and obtain
\[
\delta_h \approx - \sqrt{N_h}(\sqrt{N_h} - \sqrt{N_e}), \quad (16)
\]
\[
\delta_e \approx - \sqrt{N_e}(\sqrt{N_h} - \sqrt{N_e}). \quad (17)
\]
From this we can find that \((\delta_h + \delta_e) \approx (\sqrt{N_h} - \sqrt{N_e})^2\) is always positive regardless whether \(N_h > N_e\) or \(N_h < N_e\). Therefore, the actual \(T_c\) reduction should be slower than the \(d\)-wave case. How much slower will be determined by the magnitude of \((\delta_h + \delta_e)\) compared to \(1\) (\(s\)-wave limit) and \(0\) (\(d\)-wave limit).

From the relation \((\delta_0 + \delta_{h,e}) \approx (\sqrt{N_h} - \sqrt{N_e})^2\) we can guess that the the \(T_c\) suppression rate is rather close to the \(d\)-wave case because the quantity \((\delta_0 + \delta_e)\) is \(\ll 1\) unless the difference of the DOSs between the bands is unrealistically large. In reality, there are more than two bands and also the intra-band interactions – which was neglected in the above analysis – would make a simple analysis rather difficult. However, a practical rule of thumb is that the \(T_c\) suppression rate by non-magnetic impurities in the \(\pm s\)-wave state should be quite similar to the \(d\)-wave case. We will show the numerical results obtained by directly solving the gap Eqs. (1) and (2) below.
Magnetic Impurity Case – Let us now turn to the magnetic impurity scattering case. For magnetic impurities, if we assume only an exchange coupling such as $S \cdot \hat{\sigma}$ (where $S$ is the momentum of the impurity atom and $\hat{\sigma}$ is the spin of the electrons), we can draw a simple result from the above analysis. Because the exchange coupling flips the spin part of the singlet wave function [12], the result of the magnetic impurity scattering is to change the sign of $\Delta_0$ in the numerator of Eq. (11). The final result in the reduced gap equation is to replace $\Delta_0$ by $-\Delta_0$ but keeping $\Gamma$ the same in Eq. (13). For the non-magnetic impurities for the $\pm$s-wave pairing, we had the relation

$$ (1 + \delta_e)(1 + \delta_h) > 1. $$

(18)

It is equal to 1 for a $d$-wave pairing state. Eq. (13) was the very reason why the non-magnetic impurity suppression rate in the $\pm$s-wave state is slower than the $d$-wave case.

Now, for the magnetic impurity scattering, we have, as discussed above

$$ (1 - \delta_e)(1 - \delta_h) < 1. $$

(19)

It is then immediately clear that the magnetic impurity suppression rate of $T_c$ for $\pm$s-wave pairing should be faster than the $d$-wave case. For realistic parameter values, the suppression rates are, as shown in Figs. 1 and 2 from numerical calculations, only marginally faster than the $d$-wave state. In Fig. 3 we used exaggerated parameter values to demonstrate this the point more clearly. This result, however, is only of an academic interest because most of magnetic impurity atoms would have a much larger potential interaction than the exchange interaction.

Numerical Results – With the typical band structure of the Fe-based pnictides [13], we obtained $N_0(0)/N_e(0) \approx 2.6$ in the previous calculations of Ref. [11]. With this realistic parameter and all interactions included, Fig.1 shows the calculation results of normalized critical temperatures $T_c/T_c^0$ vs normalized impurity scattering strength $\Gamma/k_BT_c$ for $c=0$. The calculations are with the realistic bands $N_0/N_e \approx 2.6$ and with the full calculations are with the realistic bands $N_0/N_e \approx 2.6$ and with the interband interactions $V_{he}$ and $V_{eh}$ only.

FIG. 1: (Color online) Normalized critical temperature $T_c/T_c^0$ vs normalized impurity scattering strength $\Gamma/k_BT_c^0$ ($c=0$). The calculations are with the realistic bands $N_0/N_e \approx 2.6$ and with the full interactions $V_{hh}, V_{ee}, V_{he}$ and $V_{eh}$.

FIG. 2: (Color online) Normalized critical temperature $T_c/T_c^0$ vs normalized impurity scattering strength $\Gamma/k_BT_c^0$ ($c=0$). The calculations are with the realistic bands $N_0/N_e \approx 2.6$ and with the interband interactions $V_{he}$ and $V_{eh}$ only.

FIG. 3: (Color online) Normalized critical temperature $T_c/T_c^0$ vs normalized impurity scattering strength $\Gamma/k_BT_c$ in the unitary limit scattering ($c=0$). Weaker limit of impurity scattering, for example, with $c=1$ would just yields twice slower suppression rate. As can be seen, there are almost no differences among all three cases. This is consistent with our analytic analysis because $(\delta_h + \delta_e) \approx 0.104 \ll 1$ in this case. Note that the normalization of the impurity scattering strength $\Gamma$ by $T_c^0$ instead of using the gap values $\Delta_0$ at $T = 0$ is for convenience for comparison with future experiments. Also the fact that $\Gamma/k_BT_c \sim 1$ when $T_c/T_c^0 \to 0$ is a pure coincidence of the parameter choice, which is clear in Fig.3.
In Fig. 2, we artificially shut down the intraband interactions $V_{hh}$ and $V_{ee}$; without the intraband repulsions $T_0^c$ itself increases by about 40%. But the normalized $T_c/T_0^c$ vs the impurity scattering strength $\Gamma/k_B T_0^c$ are indistinguishably the same as the case of Fig. 1. This result shows that our main analytic analysis for the $T_c$ suppression with the interband interaction only will be valid for more complicate multiband model in general.

In Fig. 3, we artificially increase the DOS ratio to $N_h/N_e = 9$ which is of course unrealistic ratio; this unrealistic parameter yields $(\delta_h + \delta_e) \approx 0.4$. The calculations demonstrate that the suppression rate of $T_c$ indeed follow the trend that we found from the analytic estimation. It also demonstrates that in realistic case the $T_c$ suppression of the $\pm s$-wave state by either magnetic or non-magnetic impurities should be indistinguishably close to the case of the standard d-wave SC.

Conclusions – In summary, we studied the effect of impurities for the $T_c$ suppression on the $\pm s$-wave SC using a generalized $\sigma$-matrix method. The main finding is that despite a possibly large difference of the positive and negative s-wave OP magnitudes, the $T_c$ suppression rate is practically indistinguishable from the standard d-wave case. This is because the DOS enters together with the OP for the scattering process. As a by-product, we found the subtle difference between the magnetic and non-magnetic impurities for the $T_c$ suppression, which should, however, be a quite small difference in realistic case.

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[1] Y. Kamihara et al., J. Am. Chem. Soc. 128, 10012 (2006); Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc. 130, 3296 (2008).

[2] Phys. Today 61, Issue 5, 11 (2008); G. F. Chen et al., Phys. Rev. Lett. 100, 247002 (2008); G. F. Chen et al., Nature 453, 761 (2008).

[3] I.I. Mazin, D.J. Singh, M.D. Johannes, M.H. Du, Phys. Rev. Lett. 101, 057003 (2008).

[4] H.-Y. Choi and Y. Bang, arXiv:0807.3404

[5] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. 3, 552 (1959).

[6] M. J. Rice, H. Y. Choi, and Y. R. Wang, Phys. Rev. B 44, 10414 (1991).

[7] L. Malone et al., arXiv:0805.3908 (unpublished); K. Hashimoto et al., Phys. Rev. Lett. 102, 017002 (2009); C. Martin et al., arXiv:0807.0876 (unpublished).

[8] K. Matano et al., Europhys. Lett. 83, 57001 (2008); H.-J. Graf et al., Phys. Rev. Lett. 101, 047003 (2008); H. Mukuda et al., J. Phys. Soc. Jpn. 77 (2008) 093704; Y. Nakai et al., J. Phys. Soc. Jpn. 77 (2008) 073701.

[9] Y. Bang and H.-Y. Choi, Phys. Rev. B 79, 054529 (2009).

[10] D. Parker, O.V. Dolgov, M.M. Korshunov, A.A. Golubov, I.I. Mazin, Phys. Rev. B 78, 134524 (2008); A.V. Chubukov, D. Efremov, I. Eremin, Phys. Rev. B 78, 134512 (2008); M. M. Parish, J. Hu, B. A. Bernevig, Phys. Rev. B 78, 134512 (2008).

[11] Y. Bang and H.-Y. Choi, Phys. Rev. B 78, 134523 (2008).

[12] A.A. Abrikosov and L.P. Gorkov, Sov. Phys. JETP, 12, 1243 (1961).

[13] D.J. Singh and M.-H. Du, Phys. Rev. Lett. 100, 237003 (2008); C. Cao, P. J. Hirschfeld, H. Cheng, Phys. Rev. B 77, 220506 (2008); E. Manousakis, Jun Ren, E. Kaxiras, Phys. Rev. B 78, 205112 (2008).