A real space approach to study the effect of disorder on the $\pm s$-wave state of the iron-based superconductors.

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In this work we have developed a real space based approach to study the effect of disorder on a model two band Hubbard Hamiltonian which represents a “$\pm s$-wave superconductor”. A iron- pnictide superconductor has this symmetry of superconducting order parameter. Using our method we analyse the effect of substitutional disorder on diagonal and off-diagonal terms of the Hamiltonian of the system. We find that if the form of the intraband pairing potential is nonlocal then superconductivity survives even when the repulsive interband interaction is dominant. Disorder in the interband intersite hopping integral is seen to kill superconductivity in the system. Thus such randomness leads us to a paradigm beyond Anderson’s proposition for “dirty superconductors”

I. INTRODUCTION

The exploration of “unconventional superconductivity” (superconductivity whose microscopic origin can not be explained by BCS theory) in Fe-based superconductors was triggered by the discovery of $T_c=26$ K in LaFeAsO$_{1-x}$F$_x$ ($x=0.05-0.12$) in 2008[1]. Eventually the critical temperature could be raised to 56K (for Sm doped SrFeAsF) under high pressure [2]. The phase diagrams for certain systems like Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$[3] or SmFeAsO$_{1-x}$F$_x$[4, 5] shows the coexistence of long ranged magnetic order and superconductivity for a narrow concentration regime. Unlike cuprates, here atomic disorder in the superconducting Fe layer does not suppress superconductivity. But optimum $T_c$ is obtained at concentration regimes where the magnetic order is destroyed. For certain other systems like CeFeAsO$_{1-x}$F$_x$[6] superconducting order develops only at concentration regimes where magnetic order gets completely destroyed.

These systems have a discontinuous sign change of the order parameter (OP) phase between bands. This OP symmetry was analysed first for LaFeAsO$_{1-x}$F$_x$ compound by Mazin et al[7]; Boeri et al [8]; Cao et al [9]; Ma et al [10] showed that Fe 3d orbitals contribute the major spectral weight near the Fermi Surface. The $k$ space picture reveals the presence of 2 hole circles around the $\Gamma$ (0,0) point (involving Fe $d_{xz}$ and $d_{yz}$ bands) and 2 co-centered elliptical electron pockets around the $M$ ($\pm \pi,\pm \pi$) point (formed by hybridization of $d_{xy}$ and $d_{yz}$ bands). The fermiology in the said LaFeAsO$_{1-x}$F$_x$ compound shows strong but broad AFM spin fluctuation near $M$ point in the Brillouin zone. These fluctuations, while too broad to induce a magnetic instability, is instrumental in creating a superconducting state with OP of opposite signs on electron and hole pockets.

The pair potential for the hole band is provided by the electron band and vice versa for this system. Thus the band with larger DOS near the Fermi Level should interestingly govern the physics of the system but hold a smaller gap ! This indicates that the OPs, the critical temperature $T_c$ and the response to disorder would be very unconventional indeed.

In order to model Fe-based superconductors, a study done by Bang et al[11] used a “phenomenological two-band model” for the system. To represent the appropriate physics in the simplistic possible way they used just one hole band around $\Gamma$ and one electron band around $M$ point. Here two kinds of OP symmetry leading to sign changing gaps between two bands is possible. One is the usual i) $\pm s$-wave symmetry and the other is the ii) double d-wave gap where each band has a d-wave gap but there is a $\pi$ phase shift between two bands. Using similar parameters they showed that the $\pm s$-wave gap is energetically more favourable and thus more realizable in systems with FeAs-like gap.

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II. METHODOLOGY

A. Hubbard model for ± s-wave

To study the effect of disorder on a multi-band ± s-wave superconducting system we shall begin with the simplest model, namely, the two band percolating Cooper-pair in model lattices. The Hamiltonian is given by:

\[ H = -\sum_{<i,j>,m,m'} \sum_{\sigma} t_{im,jm} c_{im}\sigma c_{jm}\sigma + \sum_{i,m,\sigma} (\varepsilon_{im} - \mu)n_{im\sigma} - \sum_{<i,j>,m} |U_{mm}(ij)|n_{im\uparrow}n_{jm\downarrow} + \sum_{i,m,m',\sigma,\sigma'} |U_{mm'}(i)|c_{im\sigma}'c_{im\sigma}c_{im'\sigma}c_{im'\sigma}' \tag{1} \]

In Eqn.1 \( c_{im\sigma}' \) is the usual electron creation and annihilation operators for orbital (band) \( m \), with spin \( \sigma \) in site labeled by \( i \) of a square or cubic lattice. The index \( m \) runs over the two bands labeled by \( s \) and \( l \), \( \mu \) is the chemical potential and \( \varepsilon_{im} \) is the local on-site energy at the site labeled by \( i \) in the band \( m \). The hopping integral \( t_{im,jm} \) has four components: a) \( t_{is,js} = t_s \) is the hopping integral for \( s \) band from \( i \) to its nearest neighbour \( j \), b) \( t_{it,jl} = t_l \) is the hopping integral for \( l \) band from a site \( i \) to its nearest neighbour \( j \). The interband hopping integrals are c) \( t_{is,jl} = t_{il}^\dagger \) is the hopping integral from a site \( i \) in the \( s \) band to one of its nearest neighbours \( j \) in the \( l \) band (or vice-versa) and d) \( t_{is,lt} = t_{sl} \) is the interband hopping integral.

Both intraband and interband interaction is included in our model Hamiltonian. It is to be noted that the interband interaction term is a pair tunneling term from the \( s \)-band to the \( l \)-band. The intraband interaction \[ U_{mm'}(ij) \] is attractive and the interband interaction \[ U_{mm'}(ij)' \] is repulsive. The intraband interaction can be local or non-local (but not sign changing) leading to ± s-wave superconductivity.

B. Treatment of disorder: Augmented space formalism

We shall mainly focus on the binary alloy kind of systems, where a randomness is present on the on-site energy term. This kind of disorder affects only the diagonal terms of the Hamiltonian. Let us think of a binary AB alloy, where A and B are the constituent atoms of the system with on-site energy \( \varepsilon_A \) and \( \varepsilon_B \) respectively. We also introduce a site occupation variable \( n_i \) which has the value either 0 or 1. If \( n_i = 1 \), then site will be occupied by A atom and if it is 0 then site will be occupied by B. So on-site energy of the system can be written as,

\[ \varepsilon_i = \varepsilon_A n_i + \varepsilon_B (1-n_i) = \varepsilon_B + \delta \varepsilon n_i \tag{2} \]

We shall define disorder strength \( D \) as, difference between on-site energy terms i.e \( D = (\varepsilon_A - \varepsilon_B) \). Probability density of \( n_i \) for the system can be written as,

\[ p(n_i) = x\delta(n_i-1) + y\delta(n_i) \tag{3} \]

where \( x \) and \( y \) is the concentration of the A and B atom in the system respectively. Since \( n_i \) in this system has only two values so configuration space \( \langle \phi_i \rangle \) of \( n_i \) has rank 2. \( \phi_i \) spanned by the states \( |A_i \rangle \) and \( |B_i \rangle \). In augmented space formalism we map every random variable \( n_i \) to a an operator \( \tilde{N}_i \) such that \( \tilde{N}_i \) acting with \( \phi_i \) give probability density as its spectral density. Spectral density of the system is given by,

\[ p(n_i) = -\frac{1}{\pi} \lim_{\eta \to 0} \Im \langle \phi_i | \{ (n_i + i\eta)\tilde{I} - \tilde{N}_i \}^{-1} | \phi_i \rangle \tag{4} \]

\( \tilde{N}_i \) has the eigenvalues same as the eigenvalues taken randomly by \( n_i \), corresponding to the eigenfunctions \( |A_i \rangle \) and \( |B_i \rangle \). Here \( |\phi_i \rangle = \sqrt{x} |A_i \rangle + \sqrt{y} |B_i \rangle \), is known as average state. The state associates with one fluctuation at \( it^\text{th} \) site is given by, \( |\eta_i \rangle = \sqrt{x} |A_i \rangle - \sqrt{y} |B_i \rangle \).

We can represent \( \tilde{N}_i \) in the above basis as,

\[ \tilde{N}_i = x + (y-x)\gamma_1^\dagger \gamma_1 + \sqrt{xy} \gamma_1^\dagger \gamma_1 \tag{5} \]

\[ \tilde{\varepsilon} = <\varepsilon_i>> + (y-x)\delta \varepsilon \gamma_1^\dagger \gamma_1 + \sqrt{xy} \delta \varepsilon (\gamma_1^\dagger \gamma_1 + \gamma_1) \tag{6} \]

This is the averaged on-site energy equation for random disorder in on-site energy.

Substituting the expression of \( \tilde{N}_i \) in equation(6) we get,

\[ \tilde{\varepsilon} = <\varepsilon_i>> + (y-x)\delta \varepsilon \gamma_1^\dagger \gamma_1 + \sqrt{xy} \delta \varepsilon (\gamma_1^\dagger \gamma_1 + \gamma_1) \tag{7} \]

This is the averaged on-site energy equation for random disorder in on-site energy.

III. RESULTS AND DISCUSSIONS

A. Ordered Situation

In this section we shall present results on ordered two-band superconductors (for ±s-wave) on square lattice with both intraband and interband Hubbard interaction. For all the calculations half filling of the states is maintained for particle-hole symmetry. Also we do not consider the interband intersite hopping term in this subsection.

For our model Hamiltonian hopping integrals are chosen as: \( t_s = 1.0 \) and \( t_l = 0.5 \) for \( s \) and \( l \) band respectively for nearest neighbour. Inter band hopping is set to zero, i.e. \( t_{sl} = 0.0 \). Partial densities of states (PDOS) for s-
and l-band are shown in Fig. 1(a) for non-interacting case, i.e. \( U_s = U_l = U_{sl} = 0 \) for square lattice. The PDOS shows van Hove singularity in the band center, two flanking kink singularities and square root singularities at the band edges which matches with standard calculation using Blochs’s theorem for ordered square lattice. Band width of the PDOS of s-band is wider because of bigger hopping amplitude.

![PDOS for s- and l-band](image)

FIG. 1: Study of superconductivity in an ordered square lattice (a) for non-interacting case, (b) for local \( \pm s \)-wave paring and (c) for non-local \( \pm s \)-wave paring case.

Next we investigate the situation in the presence of both intraband and interband interactions. Here intraband interactions can be local as well as non-local, attractive and fixed at \( U_s = -3.5 \) and \( U_l = -3.5 \). The interband interaction is local but nature of the intraband interaction should be repulsive in order to observe \( \pm s \)-wave superconductivity. In Fig. 1(b) PDOS has been shown for \( U_{sl} = 2.5 \) where \( U_s \) and \( U_l \) are local. Superconducting gap in both the bands signifies superconductivity for both the channel. This kind of superconductivity survives when the magnitude of intraband interactions are bigger than interband interaction. In Fig. 1(c) PDOS has been shown for \( U_{sl} = 4.5 \) where \( U_s \) and \( U_l \) are non-local. Here also superconductivity can be observed for both the channel. This kind of superconductivity survives even when the magnitude of intraband interactions are smaller than interband interaction.

![Variation of order parameter](image)

FIG. 2: Variation of order parameter with magnitude of interband paring potential (a) for local \( \pm s \)-wave superconductor where interband interaction is repulsive, (b) for normal \( s \)-wave superconductor with attractive interband interaction

It will be interesting to study how OP behaves with interband interaction. Here intraband potential are set to \( U_s = -3.5 \), \( U_l = -3.5 \). Intraband interactions are restricted to be local. Now interband interaction potential \( U_{sl} \) is varied. Variation of the order parameter with the magnitude of \( U_{sl} \) has been shown in Fig. 2. \( U_{sl} \) is repulsive and attractive respectively for Fig. 2(a) and Fig. 2(b). When \( U_{sl} \) is repulsive, order parameter for s-band (\( \Delta_s \)) and l-band (\( \Delta_l \)) have opposite sign to each other but their magnitude increases with increase in magnitude of interaction potential \( U_{sl} \). Both order parameter become positive when \( U_{sl} \) is switched to be attractive. For both the cases magnitude of (\( \Delta_s \)) and (\( \Delta_l \)) do not change.

### B. Substitutionally Disordered Situation

We shall now consider two-band attractive Hubbard model for a binary substitutional alloy on a square lattice. Randomness in the onsite energy will be considered for s- or l-band, then we shall see how this randomness affect our system. We shall introduce randomness in our model Hamiltonian using Eqn. 6. Concentration is fixed at \( x = y = 0.5 \). To start with we shall discuss the effect of randomness for non-interacting case, i.e. \( U_s = U_l = U_{sl} = 0 \). We keep the hopping integral \( t_s = 1.0 \) and \( t_l = 0.3 \) for the calculation. The strength of disorder is defined as \( D_m = |\varepsilon_m^A - \varepsilon_m^B| \), where m can be s- or l-band and \( \varepsilon_m^A (\varepsilon_m^B) \) be the onsite energy for A(B) atom for a band m. PDOS of s- and l-band are shown in Fig. 3(a) and Fig. 3(b) respectively for different disorder strength. As disorder is increased we see the formation of a wedge in the PDOS corresponding to a split-band regime. Now we shall consider intercasing case where all intercation potentials are set to non zero values. Here we set intraband interaction to \( U_s = U_l = -3.5 \), intraband interaction potential is considered be local here. Interband interaction potential is set to be repulsive with \( U_{sl} = 2.5 \). PDOS for s- and l-band are shown in Fig. 3(c) and Fig.
have considered random onsite energy and set disorder and the behaviour of OP has been shown in Fig. 4. Now disorder strength is varied but Interband interaction is switched to be attractive strength. OP for s-wave superconductor with disorder. We keep the onsite s-wave pairing with disorder. We keep the onsite onsite energy and set disorder strength. At higher disorder strength slight expansion of superconducting gap can be seen in l-DOS because of the split-band effect.

In this part we shall set intraband interaction potential to be non-local with \( U_i = U_l = -3.5 \) and \( U_{st} = 4.5 \). Here also effect of disorder is similar to local ±s-wave pairing. Superconductivity survives with reduced superconducting gap. In order to study the variation of OP with increasing disorder strength two cases are considered as follows: (i) Intraband interactions are set to be local with \( U_i = U_l = -3.5 \) and interband interaction is set to be repulsive with \( U_{st} = 2.5 \). This will leads to local ± s-wave. (ii) Intraband remains same as previous but Interband interaction is switched to be attractive with same value as previous. With this condition we can see normal s-wave pairing. Now disorder strength is varied and the behaviour of OP has been shown in Fig. 4. Variation of OP for local ± s-wave pairing with disorder strength is shown in Fig. 4(a). OP decreases with increase of disorder, at higher disorder strength sign of the OP for s- and l-band is reversed but superconductivity still survives. In Fig. 4(b) OP for a normal s-wave superconductor is shown for different disorder strength. Here also value of OP reduces with increasing value of disorder strength.

Next we shall investigate the effect of random interband repulsive potential for non-local ± s-wave. Here we set non-local intraband interaction to \( U_i = U_l = -3.5 \) and interband repulsive potential to \( U_{st} = 4.5 \). Here we have considered random onsite energy and set disorder strength to \( D = 3 \). In this situation we have considered two cases as follows: (i) Here we set \( U_{st} = 4.5 \) for all the sites (ii) Here we set \( U_{st} = 4.5 \) for 50% site and set it to be zero for the other sites. DOS has been shown in Fig.5 (a) and (b). Here we see that superconductivity survives for the first case even when the interband repulsive interaction is bigger than the attractive potential but superconductivity vanishes for the second case. So, superconductivity is destroyed for random interband potential model unlike random onsite potential model.

The effect of randomness of the interband intersite pairing amplitude \( t_{ij} \) for systems with local ±s-wave pairing is also studied. Here \( U_i=U_l=-3.5\) (attractive) and \( U_{st}=1.25 \) (repulsive). The intraband inter site hopping amplitudes \( t_s=1.0 \) and \( t_l=0.75 \). In Fig 6 (a) \( t_{ij} = 0.9 \) and \( t_{ij} = 0.2 \) in all the cases except for the D=0 case. In the D=0 case the system has no randomness. Here \( t_{ij} = 0.55 \) so that the average value of \( t_{ij} \) is the same in all the cases. We see that when we put in randomness in \( t_{ij} \) and increase the diagonal disorder D after a certain point the gap in the DOS closes up just like when we put in diagonal disorder in a d-wave superconductor. In (b) we take a zoomed in view of this closing up of the gap with disorder. In (c) and (d) we have \( t_{ij} = 0.9 \) and \( t_{ij} = 0.2 \). So there is randomness in \( t_{ij} \). But here D=0.5, so we have not yet reached the limit where the system behaves like a d-wave superconductor with disorder. We keep the onsite interband hopping amplitude for A species (\( t_{si} \)) fixed at 0.6 and vary \( t_{st} \) from 0.1 to 0.6 . While decreasing randomness in \( t_{st} \) tries to increase the order parameters, the
increase in the resultant average $t_{sd}$ tries to decrease the order parameters $\Delta_s$ and $\Delta_l$. So it is a competition between these two phenomenon that decides the behaviour of $\Delta_s$ and $\Delta_l$.

![Graph](image)

**FIG. 6:** (a) DOS of a non-local $\pm s$-wave superconductor with random $t_{sd}^i$, (b) zoomed view of the superconducting gap, (c) and (d) variation of order parameter for s- and l-band respectively with random $t_{sd}^i$.

### IV. SUMMARY AND CONCLUSIONS

In the present communication we have developed a real space approach to study the effect of substitutional disorder on a model multi band (orbital) superconducting system in real space. While the inter-orbital pairing is repulsive, the intra-orbital pairing is attractive. We have looked into what happens if the intra-orbital pairing is local and non-local (but without angular isotropy). For repulsive inter-orbital pairing there is a sign change of the order parameter phase between the bands which leads to pairing of electrons by pair tunneling phenomena. We have studied the effect of disorder in various situations. Randomness has been investigated in substitutionally disordered alloys where a) only 50 % sites have finite interband pairing potential $U_{sl}$, b) randomness is present only in the on-site energy (chemical disorder) and c) randomness is present only in the hopping interactions. For ordered systems two gapped situation is got in the presence of interband pairing. Only in the case where intraband pairing potential is non local then superconductivity survives when the repulsive interband potential is stronger than the attractive intraband pairing potential. The gap in one of the bands in this case is determined by the hopping integral of the other band. While randomness in the on-site energy (chemical disorder depicted by disorder strength D as defined earlier) alone can not kill superconductivity in the system, a combined effect of randomness of the interband intersite pairing potential $t_{sd}^0$ and on-site energy kills superconductivity. Thus such disorder takes us to a regime beyond the validity of Anderson’s theorem [12].

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