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

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In this work we present a real space based method to analyse the consequence of randomness on a model two band Hubbard Hamiltonian which represents a "± 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. 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 $Ba(Fe_{1-x}Co_x)_2As_2$[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]. It is believed that superconductivity here is mediated by spin fluctuations (SF). SF can lead to triplet superconductivity or singlet one that changes sign over Fermi Surface. In order to satisfy the latter criteria it is not essential to have strong angular anisotropy of the OP (as is true for *d*-wave superconductors). It can be, and in this case it is satisfied by isotropic (*s*-wave type) pairing potential that has a sign reversal corresponding to the two Fermi Surfaces that participate in superconductivity. Although it is also multiband superconductivity, it is in principle different from that seen in MgB_2. Not only is the origin of Cooper pair formation different, but also the nature of the interaction. Here the pairing interaction is repulsive, but pairing, due to the sign reversal of OP. Similar to *d* or *p*-wave pairing, here also the OP has a nearest neighbour intraorbital attractive pairing structure in real space, thus reducing the Coulomb repulsion between pairs. First principles calculations 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 Γ (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. The said fluctuations though are too broad to cause a magnetic instability, are responsible for generating 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 Γ 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) ± 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 π phase shift between two bands. Using similar parameters they showed that the ± 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 analyse the consequence of randomness on a multi-band ± s-wave superconductor we look into the simplest model, namely, the two band percolating Cooper-pair in model system lattices. The corresponding Hamiltonian is:

$$\begin{aligned}\mathbf{H} &= -\sum_{<i,j>}\sum_{m,m',\sigma} t_{im,jm'} c^{\dagger}_{im\sigma} c_{jm'\sigma} \\ &+ \sum_{i,m,\sigma}(\varepsilon_{im}-\mu) n_{im\sigma} - \sum_{<i,j>,m} |U_{mm}(ij)| n_{im\uparrow} n_{jm\downarrow} \\ &+ \sum_{i}\sum_{m,m',\sigma,\sigma'} |U_{mm'}(i)| c^{\dagger}_{im\sigma} c^{\dagger}_{im\sigma'} c_{im'\sigma} c_{im'\sigma'}\end{aligned} \tag{1}$$

In Eqn.1 $c^{\dagger}_{im\sigma}$, $c_{im\sigma}$ are the electronic creation and annihilation operators for obrbital (band) m, with spin σ in site depicted by i of a two-dimensional (square) lattice. The index m runs over the two bands labeled by s and l, μ is the chemical potential and ε_{im} is the 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) $t_{il,jl} = t_l$ is the hopping integral for l band from a site i to its nearest neighbour j. The interband hopping intergrals are c) $t_{is,jl} = t^{ij}_{sl}$ 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) $t_{is,il} = t_{sl}$ 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 $[U_{mm'}(i)]$ 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 ε_A and ε_B respectively. We also introduce a site occupation variable n_i which has the value either 0 or 1. If n_i is 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,

$$\begin{aligned}\varepsilon_i &= \varepsilon_A n_i + \varepsilon_B(1-n_i) \\ &= \varepsilon_B + \delta\varepsilon n_i\end{aligned} \tag{2}$$

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 (ϕ_i) of n_i has rank 2. ϕ_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 $\widetilde{N}_i$ such that $\widetilde{N}_i$ acting with ϕ_i give probability density as its spectral density. Spectral density of the system is given by,

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

$\widetilde{N}_i$ has the eigenvalues same as the eigenvalues taken randomly by n_i, corresponding to the eigenfunctions $\mid A_i\rangle$ and $\mid B_i\rangle$. Here $\mid \emptyset_i\rangle = \sqrt{x} \mid A_i\rangle + \sqrt{y} \mid B_i\rangle$, is known as average state. The state associates with one fluctuation at i^{th} site is given by, $|1_i\rangle = \sqrt{y}|A_i\rangle - \sqrt{x}|B_i\rangle$.

We can represent $\widetilde{N}_i$ in the above basis as,

$$\widetilde{N}_i = x + (y-x)\gamma^{\dagger}_i\gamma_i + \sqrt{xy}(\gamma^{\dagger}_i\gamma_i) \tag{5}$$

$$\widetilde{\varepsilon} = << \varepsilon_i >> + (y-x)\delta\varepsilon\gamma^{\dagger}_i\gamma_i + \sqrt{xy}\delta\varepsilon(\gamma^{\dagger}_i + \gamma_i) \tag{6}$$

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

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

$$\widetilde{\varepsilon} = << \varepsilon_i >> + (y-x)\delta\varepsilon\gamma^{\dagger}_i\gamma_i + \sqrt{xy}\delta\varepsilon(\gamma^{\dagger}_i + \gamma_i) \tag{7}$$

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

III. RESULTS AND DISCUSSIONS

A. Ordered Situation

Now, we will discuss the results on non-random two-band superconducting systems (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 $t_l = 0.3$ 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.

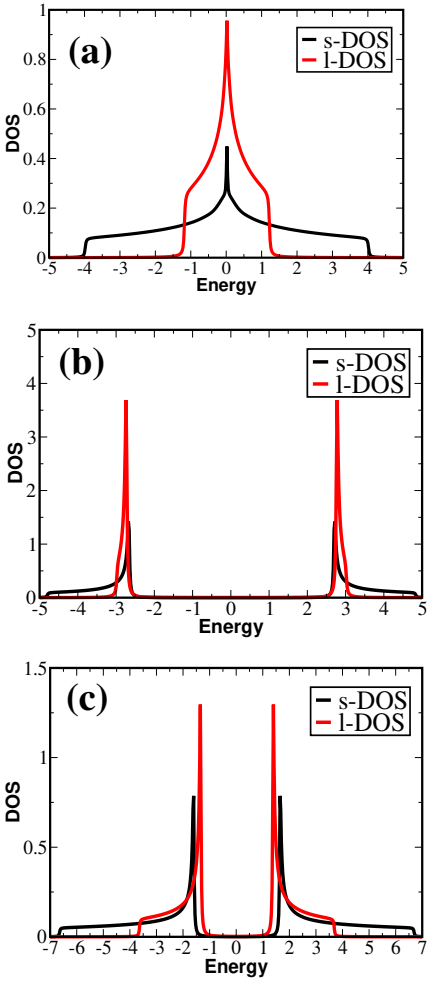

FIG. 1: Study of superconductivity in an ordered square lattice (a) for non-interacting case, (b) for local ±s-wave paring and (c) for non-local ±s-wave pairing case.

We proceed to study the system when both intraband and interband interactions are present. 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 interband interaction should be repulsive in order to observe ±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 interctions 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 interctions are smaller than interband interaction.

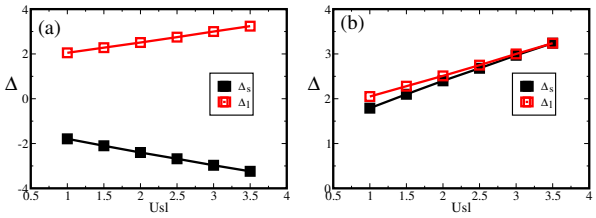

FIG. 2: Variation of order parameter with magnitude of interband paring potential (a) for local ±s-wave superconductor where interband interaction is repulsive, (b) for normal s-wave superconductor with attractive interband interaction

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 (Δ_s) and l-band (Δ_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 (Δ_s) and (Δ_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 disorder strength 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 Figure 3(a) and Figure 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 intercating case where all intercation potentials are set to non zero values.

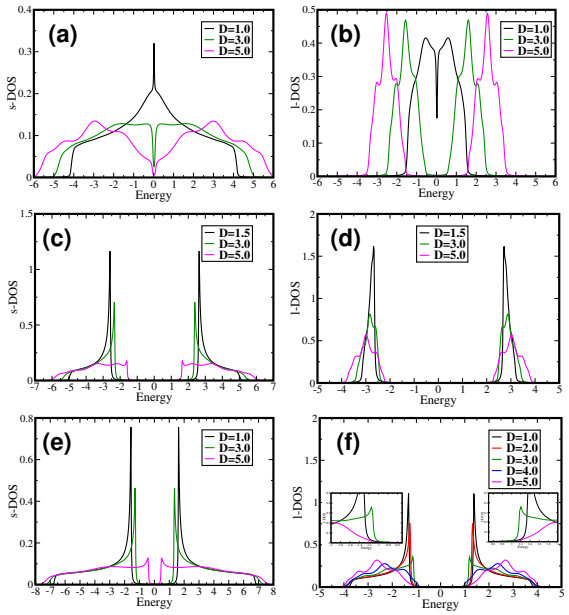

FIG. 3: DOS for different values of disorder strength (a)and(b) for non-interacting s- and l-band. (c)and (d) for local $\pm$s-wave superconductor for s- and l-band. (e) and (f)for non-local $\pm$s-wave superconductor for s- and l-band

Here we set intraband interaction to $U_s = U_l = -3.5$, intraband interation 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. 3(d) respectively. Superconductivity survives with increasing disorder strength as OP reduces with increasing value of disorder strength. At higher disorder strength slight expansion of superconducting gap can be seen in l-DOS because of the split-band effect.

The effect of randomness of the interband intersite pairing amplitude t_{sl}^{ij} for systems with local +/- s-wave pairing is also studied. Here U_s=U_l=-3.5(attractive) and U_{sl}=1.25 (repulsive). The intraband inter site hopping amplitudes t_s=1.0 and t_l=0.75. In Fig 4 (a) $t_{sl}^{ij\ a}$=$t_{sl}^{ij\ b}$=0.9 and $t_{sl}^{ij\ ab}$=0.2 in all the cases except for the D=0 case. In the D=0 case the system has no randomness. Here $t_{sl}^{ij\ a}$=$t_{sl}^{ij\ b}$=$t_{sl}^{ij\ ab}$=0.55 so that the average value of t_{slij} is the same in all the cases. We see that when we put in randomness in t_{slij} 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 $t_{sl}^{ij\ a}$=$t_{sl}^{ij\ b}$=0.9 and $t_{sl}^{ij\ ab}$=0.2. So there is randomness in t_{sl}^{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_{sl}^{a}) fixed at 0.6 and vary t_{sl}^{b} from 0.1 to 0.6 . While decreasing randomness in t_{sl} tries to increase the order parameters, the increase in the resultant average t_{sl} tries to decrease the order parameters Δ_s and Δ_l. So it is a competition between these two phenomenon that decides the behaviour of Δ_s and Δ_l.

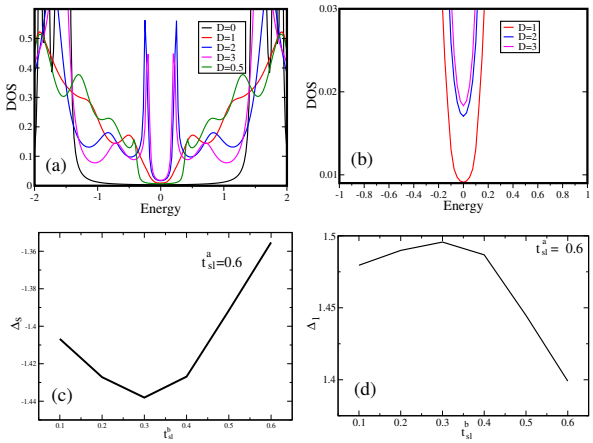

FIG. 4: (a) DOS of a non-local $\pm$s-wave superconductor with random t_{sl}^{ij}, (b) zoomed view of the superconducting gap, (c) and (d) variation of order parameter for s- and l-band respectively with random t_{sl}^{ij}

IV. SUMMARY AND CONCLUSIONS

In the present communication we present a real space approach to analyse the consequence of substitutional disorder on a model multi band (orbital) superconducting system in real space. While the inter-orbital pairing is repulsive, the intra-orbital coupling is attractive. We have looked into what happens if the intra-orbital coupling 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) randomness is present only in the on-site energy (chemical disorder) and b) randomnes 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_{sl}^{ij} 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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