A study of superconductivity in multi-band disordered systems : A vector recursion approach.

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We present a vector recursion based approach to study the effect of disorder on superconductivity in a system modeled by two-band attractive Hubbard Model. We use the augmented space formalism for the disorder averaging. In the presence of only intraband pairing in a two band disordered system with disorder in either or both bands, our calculations reveal that the gap survives in the quasiparticle spectrum; similar to single band systems. However for interband pairing the gap in the quasiparticle spectrum ceases to exist beyond a critical value of the disorder strength. In the presence of both interband and intraband pairing interaction, depending on the relative magnitude of the pairing strength, only a particular kind of pairing is possible for a half-filled two band system.

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I. INTRODUCTION

The study of superconductivity in multi-band systems has received considerable interest recently because of the discovery of superconducting materials where the Fermi surface is dominated by several bands. Examples include MgB_2 where the Fermi surface is determined by the σ and π bands arising from the B-p orbitals. It is now confirmed that the superconductivity in this material can be explained with the Bardeen-Cooper-Schrieffer (BCS) theory with two different superconducting gaps in agreement with experiments[1]. A description of unusual $p-$wave superconductivity in Sr_2RuO_4 also necessitates a multi-band model for superconductivity[2,3]. Very recently the discovery of superconductivity in Fe pnictides, whose Fermi surface is built out of the t_{2g} orbitals of Fe, has again emphasized the importance of the study of superconductivity in multi-band systems[4,5].

The complex problem of superconductivity in multi-band systems was first studied by Suhl *et al.*[6] using a tight-binding model Hamiltonian with two bands. The model included intra-band pairing and also the inter-band hopping of pairs of electrons belonging to the same band. They showed that pairing could occur in each band and, because electron-phonon interactions may have different strengths in different bands, this can give rise to two different superconducting gaps. But in the special case of only inter-band scattering, a single gap was found to be present in the density of states unless the band dispersion of the two bands had different shapes[7]. A similar model was also investigated by Machida *et al.*[8] for the study of superconductivity in multi-band systems. Recently Moreo *et al.*[9] revisited the theory of superconductivity in multi-band systems in the context of Fe pnictides. In particular they have emphasized the importance of inter-band pairing in multi-band systems in which, in contrast to earlier studies[6,8], Cooper pairs are formed by electrons belonging to two different bands. The calculations by Moreo *et al.*[9] revealed that three different regions can result from a purely inter-band pairing as a function of the interaction parameter: (i) a normal regime where the ground state is not superconducting ; (ii) an exotic superconducting "breached" regime where one of the bands is gapped at the Fermi level while the other is not, and (iii) a superconducting regime resembling the BCS states, at large attractive coupling. The existence of an exotic superconducting "breached" regime with both gapped and gapless quasiparticle excitations was also discussed by Liu and Wilczek[10] in the context of cold atoms and quantum chromodynamic systems.

The preceding discussion suggests that superconductivity in multi-band systems is not only interesting but markedly different from its single-band counterpart. In this context it will also be important to understand the role of disorder in multi-band superconducting systems since disorder is an important factor that has a profound impact on superconductivity. While the effect of disorder on superconductivity in single-band systems have been actively investigated, there are very few systematic studies of the role of disorder in multi-band systems.

The effect of disorder in single-band systems is usually discussed within the framework of Anderson's theorem[11].

For s-wave superconductors Anderson's theorem guarantees the survival of an absolute gap in the quasi-particle spectrum of the system provided the perturbation due to disorder preserves time reversal invariance and the coherence length is long enough to ensure that the pairing amplitude Δ does not fluctuate. There exists a body of work where the Bogoliubov-de Gennes (BdG) equations[12] which provide a natural framework for a fully microscopic description of the phenomena of superconductivity have been solved in conjunction with the mean-field single-site coherent potential approximation (CPA)[13–15], in order to understand the physics of superconductivity in single-band disordered systems.

Recently we have proposed an efficient real-space scheme to solve the BdG equations for single-band disordered attractive Hubbard models[16]. The aim of this paper is to propose a real space, vector recursion based approach to study the effect of disorder on a multi-band attractive-U Hubbard model where the configuration averaging, as in our earlier study, will be based on the augmented space recursion (ASR) formalism introduced by one of us[17]. The ASR gives us the flexibility of introducing the effects of random configuration fluctuations in the local environment of a site. It does not violate analytical properties of the configuration-averaged Green's function, which form an essential ingredient of the solution. It can deal easily with the effect of either off-diagonal disorder or inhomogeneous disorder such as clustering, segregation, and short-ranged ordering which usually occur intrinsically in most disordered materials due to different chemical affinities of the constituents.

We shall begin by studying superconductivity in an ordered two-band, tight-binding, attractive-U Hubbard model, using our vector recursion technique. Then, having satisfied ourselves with the reliability of our methodology, we shall proceed to study the effect of disorder on the same model. The rest of the paper is organized as follows : in Section II we shall discuss our method in some detail. Section III will be devoted to results and discussions for multi-band ordered and disordered systems. Finally in Section IV we will summarize our study.

II. METHODOLOGY

A. The multi-band attractive-U Hubbard model

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 attractive Hubbard Hamiltonian in model lattices. The Hamiltonian is given by :

$$\mathbf{H} = -\sum_{\langle i,j\rangle}\sum_{m,m',\sigma} t_{im,jm'}\; c^{\dagger}_{im\sigma}c_{jm'\sigma} + \sum_{i,m,\sigma}(\varepsilon_{im}-\mu)n_{im\sigma} - \sum_{i,m}|U_{mm}(i)|n_{im\uparrow}n_{im\downarrow} - \sum_{i}\sum_{m,m',\sigma,\sigma'}|U_{mm'}(i)|n_{im\sigma}n_{im'\sigma'} \tag{1}$$

Here m , m' are the band index. This Hamiltonian is a generalization of the single-band Hubbard Hamiltonian and similar to earlier studies by Annett *et al.*[3,18]. Our model Hamiltonian allows for both intra-band as well as inter-band pairing. The inter-band pairing term is similar to that of Annett *et al.*[3,18] and Moreo *et al.*[9] which allows Cooper pairs to be formed by electrons belonging to two different bands. The earlier studies by Suhl *et al.*[6] and Machida *et al.*[8] did not consider the pairing of electrons belonging to two different bands but a pair tunneling term given by :

$$-\sum_{i}\sum_{m,m',\sigma,\sigma'}|U^{t}_{mm'}(i)|(c_{im\sigma}c_{im\sigma'})^{\dagger}c_{im'\sigma}c_{im'\sigma'} \tag{2}$$

This term allowed for the tunneling of the Cooper pairs from one band to the other with a tunneling strength given by $U^{t}_{mm'}$.

In Eqn. (1) $\{c^{\dagger}_{im\sigma}\}, \{c_{im\sigma}\}$ are the usual electron creation and annihilation operators for orbital m with spin σ on site labelled i of a square or cubic lattice. The index m runs over the two bands labeled s and l, μ is the chemical potential and ε_{im} the local on-site energy at the site labelled i in the band m. The hopping integral $t_{im,jm'}$ has four components:: $t_{is,js} = t_s$ is the hopping integral in the s-band from a site i to one of its nearest neighbours j and $t_{il,jl} = t_l$ is that in the l-band from a site to one of its nearest neighbours. The inter-band hopping integrals are $t_{is,il} = t_{sl}$ which is the hopping integral from a site in the s-band to the same site in the l-band (or vice-versa) and $t_{is,jl} = t^{nn}_{sl}$ which 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). In this work we have not included the inter-band inter-site hopping integral t^{nn}_{sl}. However, we do consider the effect of on-site inter-band hopping integrals t_{sl} in some of our analysis. As we will see subsequently, t_{sl} will not alter the qualitative features of our results. In this model, U_{ss}=$-|U_s|$ corresponds to a local Hubbard parameter leading to a pairing interaction potential for s-band electrons and U_{ll}=$-|U_l|$ corre-

spond to a local Hubbard parameter for l-band electrons. Here, both the attractive interactions give rise to s-wave pairing since they are local. The inter-band pairing interaction $U_{mm'}$=$-|U_{sl}|$ is the local attractive potential between electrons in the s- and l- band.

The BdG mean field decomposition[12] of the interaction terms give expectation values to the intra and inter band pairing amplitudes:

$$\Delta_m = -|U_m| \ \langle c_{im\downarrow} c_{im\uparrow} \rangle \ ; \ \Delta_{sl} = -|U_{sl}| \ \langle c_{il\downarrow} c_{is\uparrow} \rangle \quad (3)$$

and also to the intra and inter band *"densities"*:

$$\langle n_{im\sigma} \rangle \ = \ \langle c_{im\sigma} c^\dagger_{im\sigma} \rangle \ ; \ \langle n_{isl\sigma} \rangle \ = \ \langle c_{il\sigma} c^\dagger_{is\sigma} \rangle \quad (4)$$

The effective quadratic BdG Hamiltonian becomes :

$$\begin{aligned} \mathbf{H}_{\text{eff}} \ = \ & -\sum_{\langle i,j \rangle} \sum_{m,m',\sigma} t_{im,jm'} \ c^\dagger_{im\sigma} c_{jm'\sigma} + \sum_{im\sigma} (\varepsilon_{im} - \hat{\mu}_{im}) \ n_{im\sigma} - \sum_{im,m',\sigma} |U_{mm'}| \frac{\langle n_{imm'\sigma} \rangle}{2} c^\dagger_{im\sigma} c_{jm'\sigma} \\ & + \sum_{im} \left(\Delta_m c^\dagger_{im\uparrow} c^\dagger_{im\downarrow} - \Delta^*_m c_{im\uparrow} c_{im\downarrow} \right) + \sum_{i,m,m'} \left(\Delta_{mm'} c^\dagger_{im\uparrow} c^\dagger_{im'\downarrow} - \Delta^*_{mm'} c_{im\uparrow} c_{im'\downarrow} \right) \end{aligned} \quad (5)$$

where $\hat{\mu}_{im} = \mu - |U_{mm}| \langle n_{im} \rangle / 2$ incorporates the site dependent Hartree shift.

This effective Hamiltonian can be diagonalized by using the Hartree-Fock-Bogoliubov (HFB)[19] transformation:

$$\begin{aligned} c_{im\uparrow} \ &= \ \sum_n [\beta_{n\uparrow} u_m(r_i, E) - \beta^\dagger_{n\downarrow} v^*_m(r_i, E)] \\ c_{im\downarrow} \ &= \ \sum_n [\beta_{n\downarrow} u_m(r_i, E) + \beta^\dagger_{n\uparrow} v^*_m(r_i, E)] \end{aligned} \quad (6)$$

where β and $\beta^\dagger$ are quasi-particle operators , and $u_m(r_i, E)$, $v_m(r_i, E)$ are the quasi-particle amplitudes associated with an eigen energy E_n.

In the Hartree-Fock mean-field approximation incorporating charge-order and superconducting decoupling along with the above canonical transformation we have,

$$\begin{pmatrix} H_{ss} & \Delta_s & -N_{sl} & \Delta_{sl} \\ \Delta^*_s & -H_{ss} & \Delta^*_{sl} & N_{sl} \\ -N_{ls} & \Delta_{ls} & H_{ll} & \Delta_l \\ \Delta^*_{ls} & -N_{ls} & \Delta^*_l & -H_{ll} \end{pmatrix} \begin{pmatrix} u_s(r_i, E) \\ v_s(r_i, E) \\ u_l(r_i, E) \\ v_l(r_i, E) \end{pmatrix} = E \begin{pmatrix} u_s(r_i, E) \\ v_s(r_i, E) \\ u_l(r_i, E) \\ v_l(r_i, E) \end{pmatrix} \quad (7)$$

where (the excitation eigen-value $E \geq 0$)

$$\begin{aligned} H_{mm} u_m(r_i, E) \ &= \ (\varepsilon_{im} - \hat{\mu}_{im}) \, u_m(r_i, E) - \sum_j t_m u_m(r_j, E) \\ N_{mm'} u_{m'}(r_i, E) \ &= \ \left\{ \frac{1}{2} \ |U_{mm'}| \langle n_{mm'} \rangle + t_{mm'} \right\} u_{m'}(r_i, E) + \sum_j t^{nn}_{mm'} u_{m'}(r_j, E) \end{aligned} \quad (8)$$

Here j is the nearest neighbour of i. We can express the particle densities and the pairing amplitudes in terms of the quasi-particle amplitude as

$$\begin{aligned}
\langle n_{im}\rangle &= 2\int dE|u_m(r_i,E)|^2 f(E) + |v_m(r_i,E)|^2[1-f(E)] \\
\langle n_{imm'}\rangle &= 2\int dE u_{m'}(r_i,E)u_m^*(r_i,E)f(E) + v_{m'}^*(r_i,E)v_m(r_i,E)[1-f(E)] \\
\Delta_m &= |U_m|\int dE v_m^*(r_i,E)u_m(r_i,E)f(E) - u_m(r_i,E)v_m^*(r_i,E)[1-f(E)] \\
\Delta_{mm'} &= |U_{mm'}|\int dE v_m^*(r_i,E)u_{m'}(r_i,E)f(E) - u_m(r_i,E)v_{m'}^*(r_i,E)[1-f(E)] \qquad (9)
\end{aligned}$$

where $f(E)$ is the Fermi function. A fully self-consistent solution of (7) can be obtained provided all the normal potentials ($|U_m|n_{im}$ and $|U_{mm'}|n_{imm'}$) and anomalous potentials (Δ_{im} and $\Delta_{imm'}$) are determined self consistently from Eqn. (9). The self-consistency criteria is set to 10^{-6} for calculation of all self-consistent parameters throughout the present study.

B. Treatment of disorder : augmented space formalism

The class of systems which we shall study here will be binary substitutionally disordered alloys. We shall study randomness in the diagonal site-energies, either in one of the two bands, say the l-band ($\{\varepsilon_{il}\}$); or in both the bands ($\{\varepsilon_{is}\}$ and $\{\varepsilon_{il}\}$). We shall introduce site occupation variables $\{n_i\}$ (this should not be confused with the number operator $n_{im\sigma}$) which take values 1 or 0 according to whether the site labelled i is occupied by a A-type or a B-type of atom.

$$\varepsilon_{im} = \varepsilon_m^A\, n_i + \varepsilon_m^B\,(1-n_i) = \varepsilon_m^B + \delta\varepsilon_m n_i \qquad (10)$$

where, $m = s$ or l and ε_s^A, ε_s^B and ε_l^A, ε_l^B are the possible on-site energies corresponding to the s and l band respectively. We define the strength of disorder in the band labeled m by $D_m = |\delta\varepsilon_m| = |\varepsilon_m^A - \varepsilon_m^B|$.

If the concentrations of A and B-type of atoms in the solid are x and y, then the probability density of n_i, in the absence of short range order, is given by :

$$p(n_i) = x\delta(n_i - 1) + y\delta(n_i) \qquad (11)$$

The 'configuration space' of n_i, Φ_i, has rank 2 and is spanned by the states $|A_i\rangle$ and $|B_i\rangle$ in which the parameter ε_{im} take the values ε_m^A and ε_m^B respectively.

The augmented space formalism associates with each random variable n_i an operator $\widetilde{N}_i$ acting on its configuration space Φ_i and whose spectral density is its probability density. That is :

$$p(n_i) = -\frac{1}{\pi}\lim_{\delta\to 0}\ \Im\mathrm{m}\ \langle\emptyset_i|[(n_i+i\delta)\widetilde{I} - \widetilde{N}_i]^{-1}|\emptyset_i\rangle \qquad (12)$$

where $|\emptyset_i\rangle = \sqrt{x}|A_i\rangle + \sqrt{y}|B_i\rangle$ is the so called 'reference' state. This nomenclature arises from the fact that the augmented space theorem[20] states that the matrix element in this state is the configuration average. The other basis member is $|1_i\rangle = \sqrt{y}|A_i\rangle - \sqrt{x}|B_i\rangle$ which is a state with one 'fluctuation' about the reference state at the site i. Alternatively, it is denoted by $|\{i\}\rangle$ where $\{i\}$ is the 'cardinality sequence' of sites at which there are fluctuations. The configuration states $|A_i\rangle$ and $|B_i\rangle$ are the eigenkets of $\widetilde{N}_i$ corresponding to eigenvalues 1 and 0. The representation of the operator $\widetilde{N}_i$ in the basis $\{|\emptyset_i\rangle, |i_i\rangle\}$ is

$$\begin{aligned}
\widetilde{N}_i &= xP_{\emptyset_i} + yP_{1_i} + \sqrt{xy}\left[T_{\emptyset_i,1_i} + T_{1_i,\emptyset_i}\right] \\
&= xI + (y-x)P_{1_i} + \sqrt{xy}\left[T_{\emptyset_i,1_i} + T_{1_i,\emptyset_i}\right] \qquad (13)
\end{aligned}$$

Here, I is the identity operator, P_X are the projection operators $|X\rangle\langle X|$ and T_{XY} are the transfer operators $|X\rangle\langle Y|$ and X, Y are either $\emptyset_i$ or 1_i.

Let us define a configuration fluctuation creation operator at the site labeled i as : $\gamma_i^\dagger|\emptyset_i\rangle = |1_i\rangle$. Since each site can either be $\emptyset$ or 1, this is a fermion-like creation operator with $\gamma_i^\dagger|1_i\rangle = 0$. Similarly we define a configuration fluctuation annihilation operator $\gamma_i|1_i\rangle = |\emptyset_i\rangle$ and $\gamma_i|\emptyset_i\rangle = 0$. In terms of these operators $P_{1_i} = \gamma_i^\dagger\gamma_i$ counts the number of configuration fluctuations at the site i, and of the transfer operators : $T_{\emptyset_i,1_i} = \gamma_i$ annihilates and $T_{1_i,\emptyset_i} = \gamma_i^\dagger$ creates a configuration fluctuation at the site i.

The operator $\widetilde{N}_i$ in this new representation is :

$$\widetilde{N}_i = xI + (y-x)\ \gamma_i^\dagger\gamma_i + \sqrt{xy}\ \left(\gamma_i^\dagger + \gamma_i\right) \qquad (14)$$

So,

$\varepsilon_{im} = \varepsilon_m^B + \delta\varepsilon_m\ n_i$ has associated with it an operator,

$$\tilde{\varepsilon}_{im} = \langle\varepsilon_m\rangle I + \ (y-x)\delta\varepsilon_m\ \gamma_i^\dagger\gamma_i + \sqrt{xy}\ \delta\varepsilon_m\ \left(\gamma_i^\dagger + \gamma_i\right) \qquad (15)$$

obtained by replacing n_i with its operator form $\widetilde{N}_i$ (see

eqn14) where, $\langle \epsilon_m \rangle$ refers to the average :

$$\langle \epsilon_m \rangle = x\epsilon_m^A + y\epsilon_m^B \tag{16}$$

with $m = s$ or l, $\delta\varepsilon_s = \varepsilon_s^A - \varepsilon_s^B$ and $D_s = |\delta\varepsilon_s|$, $\delta\varepsilon_l = \varepsilon_l^A - \varepsilon_l^B$ and $D_l = |\delta\varepsilon_l|$.

The augmented space theorem[20] states that the configuration average of a function of a set of independent random variables : $\mathbf{A}(\{n_i\})$ can be expressed as a matrix element in the full configuration space of the disordered system $\Phi = \prod^{\otimes} \Phi_i$,

$$\ll \mathbf{A}(\{n_i\}) \gg = \langle \{\emptyset\} | \widetilde{\mathbf{A}}(\{\widetilde{N}_i\}) | \{\emptyset\} \rangle \tag{17}$$

where $|\{\emptyset\}\rangle = \prod_i^{\otimes} |\emptyset_i\rangle$ and $\widetilde{\mathbf{A}}(\{\widetilde{N}_i\})$ is the representation of the operator $\widetilde{\mathbf{A}}$ in the configuration space Φ, constructed by replacing all random variables n_i by their corresponding operators $\widetilde{N}_i$. A compact way of representing a basis in configuration space is to denote it by the set of sites where we have a configuration fluctuation. This set is called the *cardinality set* and the meaning of the empty cardinality set $\{\emptyset\}$ then becomes obvious. For the present system the Hamiltonian contains the random variables $\{\varepsilon_{is}\}$ and$\{\varepsilon_{il}\}$. So we need to construct the Hamiltonian in the augmented space $\Psi = \mathcal{H} \otimes \prod_i^{\otimes} \Phi_i$ by replacing all the random variables ε_{is} and ε_{il} by the corresponding operators shown in Eqn. (15). The effective augmented space Hamiltonian becomes :

$$\begin{aligned}
\widetilde{\mathbf{H}}_{\text{eff}} \;=\; & -\sum_{\langle i,j\rangle,m,m',\sigma} t_{im,jm'}\; c^\dagger_{im\sigma} c_{jm'\sigma} \otimes I + \sum_{im\sigma} (\langle \varepsilon_m \rangle - \widehat{\mu}_{im}) n_{im\sigma} \otimes I + \sum_{im\sigma} \delta\varepsilon_m\; n_{im\sigma} \otimes \Big\{ (y-x)\gamma_i^\dagger \gamma_i + \sqrt{xy}(\gamma_i^\dagger + \gamma_i) \Big\} \ldots \\
& - \sum_{im,m',\sigma} |U_{mm'}| \frac{\langle n_{imm'\sigma} \rangle}{2} c^\dagger_{im\sigma} c_{jm'\sigma} \otimes I + \sum_{im} \Big(\Delta_m c^\dagger_{im\uparrow} c^\dagger_{im\downarrow} - \Delta^*_m c_{im\uparrow} c_{im\downarrow} \Big) \otimes I \ldots \\
& + \sum_{i,m,m'} \Big(\Delta_{mm'} c^\dagger_{im\uparrow} c^\dagger_{im'\downarrow} - \Delta^*_{mm'} c_{im\uparrow} c_{im'\downarrow} \Big) \otimes I
\end{aligned} \tag{18}$$

In the special case when there is randomness in just one of the bands (say l), in the Eqn.(18) we put $\delta\varepsilon_s = 0$ and $\langle \varepsilon_s \rangle = \varepsilon_s$.

After constructing the Hamiltonian in augmented space the augmented space theorem then automatically ensures that the configuration average is a projection onto the state with no 'fluctuations'[20] :

$$\ll \underline{\underline{\mathbf{G}}}(i,i,E) \gg = \langle \emptyset | \underline{\underline{\widetilde{\mathbf{G}}}}(i,i,E) | \emptyset \rangle$$

where $\underline{\underline{\widetilde{\mathbf{G}}}} = (E\underline{\underline{\tilde{I}}} - \underline{\underline{\widetilde{\mathbf{H}}}}_{\text{eff}})^{-1}$. All operators here are 4×4 matrices(here double underbar indicates 4×4 matrices) in the space spanned by the two bands and the electron-hole degrees of freedom[21] arising in BdG formalism.

The Green functions are obtained using the vector recursion technique introduced by Haydock and Godin[22,23]. The vector recursion has been described in great detail in the given references and in our earlier work[16]. We shall indicate the main points and the interested reader may refer to the quoted references for details. Once the BdG Hamiltonian is set up as in Eqn.(7) and the effective augmented space transformation carried out as in Eqn.(18), the vector recursion technique essentially changes the basis in order to block tridiagonalize the effective Hamiltonian. The basis is recursively generated :

$$|1 \gg \;=\; \begin{pmatrix} u_s(\vec{r}_i, E) \otimes \{\emptyset\} \\ v_s(\vec{r}_i, E) \otimes \{\emptyset\} \\ u_l(\vec{r}_i, E) \otimes \{\emptyset\} \\ v_l(\vec{r}_i, E) \otimes \{\emptyset\} \end{pmatrix}$$

The coefficients $\underline{\underline{A}}_n$ and $\underline{\underline{B}}_n$ are matrices and obtained from the orthogonality of the generated basis and between rows of the same basis The configuration averaged diagonal matrix element of the Green function then follows as a matrix continued fraction :

$$\ll \underline{\underline{G}}(\vec{r}_i \vec{r}_i; E) \gg = \ll 1 | \mathbf{G} | 1 \gg = \underline{\underline{G}}_0(E)$$

$$\underline{\underline{G}}_n(E) = \Big(z\underline{\underline{I}} - \underline{\underline{A}}_n - \underline{\underline{B}}^\dagger{}_{n+1} \underline{\underline{G}}_{n+1}(E) \underline{\underline{B}}_{n+1} \Big)^{-P_{n-1}}$$

$$n \;=\; 0, 1, 2, \ldots N_2 - 1$$

where A^{-P_n} denotes inverse in the subspace spanned by the basis $\{|n+1 \gg, |n+2 \gg \ldots\}$. The matrix continued fraction is terminated in two steps. The matrix coefficients $\{\underline{\underline{A}}_n, \underline{\underline{B}}_n\}$ are calculated exactly for $n < N_1$, then : first, by putting $\underline{\underline{A}}_n = \underline{\underline{A}}_{N_1}$ and $\underline{\underline{B}}_n = \underline{\underline{B}}_{N_1}$ for all $N_1 \le n < N_2$ and second, $\underline{\underline{G}}_{N_2}(E) = (E + i\eta)^{-1}\, \underline{\underline{I}}$

The physical quantities of interest (Eqn.(9)) relevant to the study can be expressed as appropriate matrix elements of the Green's function.

$$\begin{aligned}
\langle n_m \rangle &= -\frac{1}{\pi} \lim_{\eta \to 0} \text{Im} \int_{-\infty}^{\infty} \left[\mathbf{G}^{++}_{mm}(i,i,E+i\eta) f_n + \mathbf{G}^{--}_{mm}(i,i,E+i\eta)(1-f_n) \right] dE \\
\Delta_m &= -\frac{1}{\pi} \lim_{\eta \to 0} \text{Im} \int_{-E_c}^{+E_c} \left[\mathbf{G}^{+-}_{mm}(i,i,E+i\eta) f_n + \mathbf{G}^{-+}_{mm}(i,i,E+i\eta)(1-f_n) \right] dE \\
\langle n_{mm'} \rangle &= -\frac{1}{\pi} \lim_{\eta \to 0} \text{Im} \int_{-\infty}^{\infty} \left[\mathbf{G}^{++}_{mm'}(i,i,E+i\eta) f_n + \mathbf{G}^{--}_{mm'}(i,i,E+i\eta)(1-f_n) \right] dE \\
\Delta_{mm'} &= -\frac{1}{\pi} \lim_{\eta \to 0} \text{Im} \int_{-E_c}^{+E_c} \left[\mathbf{G}^{+-}_{mm'}(i,i,E+i\eta) f_n + \mathbf{G}^{-+}_{mm'}(i,i,E+i\eta)(1-f_n) \right] dE \qquad (19)
\end{aligned}$$

Where + and - refer to electron and hole spaces of the BdG formalism[21] and the energy interval $[-E_c, +E_c]$ is the short interval around the Fermi-energy of the system where the interaction has its effect.

III. RESULTS AND DISCUSSION.

A. Ordered Systems.

In this section we shall present results on ordered two band superconductors (both the bands having s-orbital character) on square and cubic lattices with both local intra and inter-band Hubbard parameters. The system is kept fixed at half-filling unless otherwise stated. Since these results are well known from other approaches, a comparison with them will ascertain the viability and numerical accuracy of our proposed methodology.

For our model system the hopping integrals are chosen as follows : in Figs.1 (a)-(d) the intra-band nearest neighbour hopping elements are t_s=1.0 and t_l=0.5 and the inter-band on-site hopping t_{sl}=0.0.

The s- and l-band partial densities of states (PDOS) for the case when $U_s = U_l = U_{sl} = 0$ for the ordered system are shown in Fig.1 (a) and (c) for the square and cubic lattices respectively. The two sets of PDOS exactly match the standard calculations using Bloch's theorem. One can clearly see in Fig.1 (a) the band-center integrable Van Hove singularity, the two flanking kink singularities and the square-root singularities at the band edges that are characteristic of a square lattice. The cubic lattice PDOS [see Fig.1 (c)] is characterized by constant DOS at the band center and terminate in kink singularities on both sides. The s-band with greater intra-band hopping integral is wider, as expected.

Next we investigate the situation in the presence of intra-band pairing, *ie.* Hubbard parameter U_s and U_l are only finite. This corresponds to the system studied by Suhl *et. al.*[6] in the absence of inter-band tunneling of electrons. Thus, U_{sl} in Eqn.(1) is set to zero. In Fig.1 (b) and (d) we consider the cases where U_s=U_l = 4.0 and the system is kept fixed at half filling. The BdG equations are solved recursively and self-consistently as described earlier. After self-consistency the superconducting order parameter Δ_s and Δ_l are found to be non-zero. The s and l configuration averaged PDOS for the system are calculated by using the relation

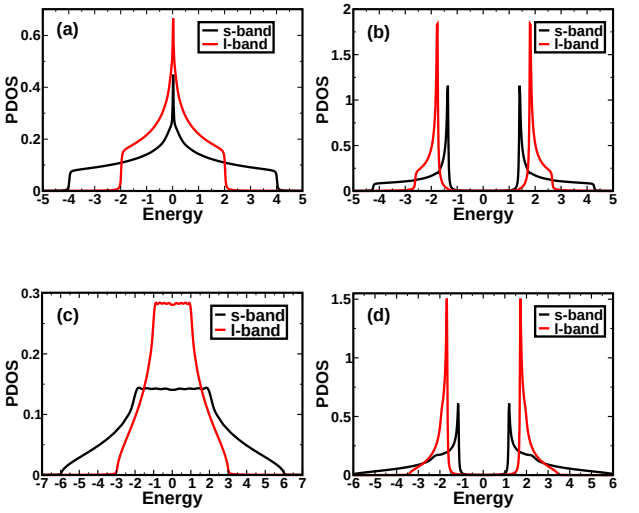

FIG. 1: (Color online) Study of superconductivity in an ordered square lattice [(a) and (b)] and cubic lattice [(c) and (d)] having two bands s and l.
(1) Intra-band hopping integrals : t_s=1.0 and t_l=0.5 and (2) Hubbard parameters for (a) and (c) are : U_s=U_l=U_{sl}=0.0 and for (b) and (d) are : U_s=U_l=4.0 and U_{sl}=0.

$$\ll n_m(E) \gg = -\frac{1}{\pi} \lim_{\eta \to 0} \Im m \ \ll G^{++}_{mm}(1,1,E+i\eta) \gg$$

where, $m = s$ or l, η is an infinitesimal positive imaginary part of the energy and + refer to the electron states in the BdG formalism.

The PDOS shown in Fig1(b) and 1(d) reveal that inspite of the parameters U_s=U_l, the superconducting pair-

ing amplitude Δ_s and Δ_l are different. This is due to the difference in band width (W) as $t_s \neq t_l$, and the observation that the effective parameters U_m/W ($m = s$ or l) are responsible for the magnitude of the gap seen in the local DOS.

In view of the above we have also investigated the situation only with intra-band Hubbard parameters such that $U_s \neq U_l$. We have considered $U_s = 3.0$ and $U_l = 1.0$. Since the effective parameter U_s/W=0.75 > U_l/W=0.5 we did find $\Delta_s > \Delta_l$. The earlier study by Suhl *et. al.*[6] had also found two different band gaps arising in a two band model system. Two different superconducting gap was later realized in MgB_2[24–30].

Next in addition to the intraband pairing we have also included interband pairing of electrons. In the presence of both inter and intra-band Hubbard parameters an interesting competitive effect sets in as can be seen from Fig.2(a). We keep the intra-band attractive Hubbard parameter fixed (U_s=U_l=2.0), and vary the inter-band Hubbard parameter U_{sl}. The intra-band hopping integrals are choosen to be t_s=1.0 and t_l=0.5 and inter-band on-site hopping integral is t_{sl}=0.2. We see (from Fig.2(a)) when U_s=$U_l \geq U_{sl}$ then it is the intra-band pairing amplitude that is only finite and the inter-band pairing amplitude vanishes. On the other hand, when U_s=$U_l < U_{sl}$ then it is only the inter-band pairing amplitude that is non-zero. Our calculations shows for momentum independent pairing in s-like bands depending on the strength of the attractive interaction, only a particular kind of pairing either intra-band or inter-band is possible for two band half-filled systems when both the bands have s-wave character.

Finally, we examine the effect of the inter-band (on-site) hopping integral t_{sl} on the pairing amplitude Δ for a half-filled system. Fig.(2)(b) and Fig.(2)(c) displays the case for dominant intraband pairing (U_s=U_l=3.5 > U_{sl}=2.0) and dominant interband pairing (U_s=U_l=2.0 < U_{sl}=3.5) respectively. We find from the figures that inclusion of intra-band on-site hopping term t_{sl} does not change the qualitative picture for a two band system except to reduce the magnitude of the gap.

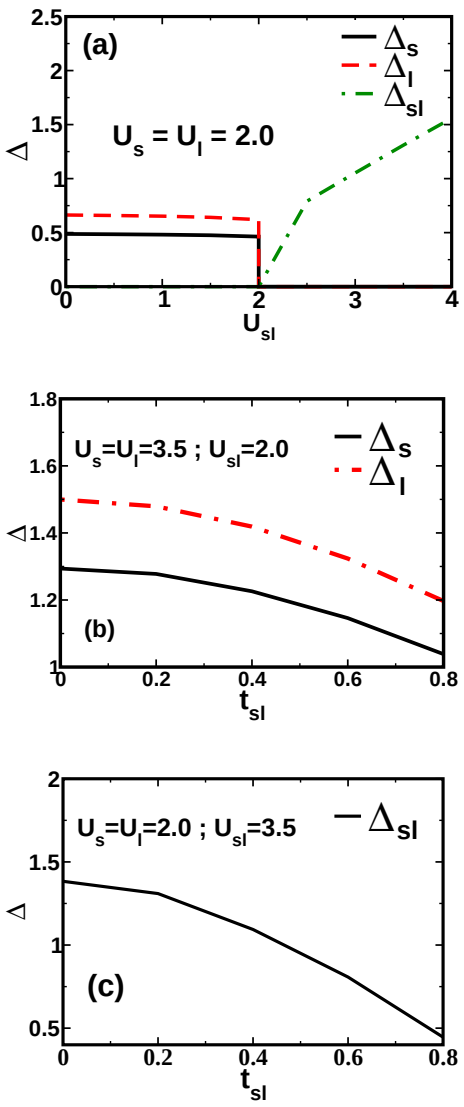

FIG. 2: (Color online) Variation of Δ for a square lattice when both intra and inter-band interaction potentials are non-zero. Here the intra-band hopping integrals are t_s=1.0 and t_l=0.5 for the s and l-bands respectively. In (a) the intra-band pairing potentials $|U_s|$ and $|U_l|$ are kept fixed at 2.0 and U_{sl} is varied. In (b) and (c) the pairing potentials are kept fixed [(b) $U_s = U_l > U_{sl}$=2.0 and (c) $U_s = U_l < U_{sl}$=3.5] and the effect of variation of inter-band on-site hopping integral t_{sl} is studied.

B. Homogeneously disordered systems.

We shall now study an attractive-U Hubbard model of a two-band, disordered, binary substitutional alloy on a square lattice. First we consider randomness in the on-site energy in one of the two channels, namely the l-channel, and study its effect on the other channel. We introduce randomness in the on-site energy using Eqn. (15) and our Hamiltonian takes the form given in Eqn. (18). The concentrations are $x = y = 0.5$ and the system is half-filled throughout the study.

To begin with, we study the systems in a situation similar to those under which we had investigated the corresponding ordered system. We keep $t_s = 1.0$ and $t_l = 0.5$ and the strength of disorder $D_l = |\varepsilon_l^A - \varepsilon_l^B| = 1$ throughout the cases considered in Fig.3.

First we study the case when the system is non-superconducting ($U_s = U_l = U_{sl} = 0.0$). From Fig.3(a) we find due to the absence of hybridization between the s and l bands the s PDOS is not affected by randomness in the l-channel. The l PDOS (Fig.3(b)), however,

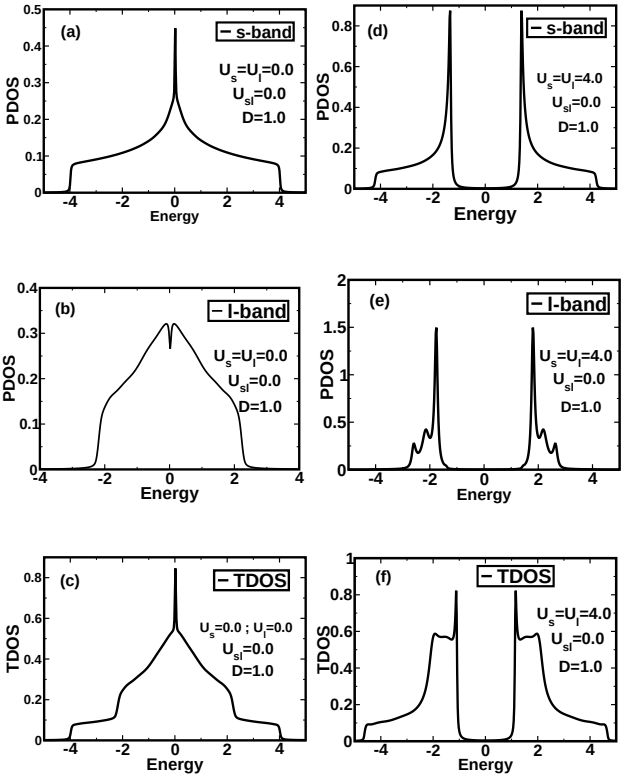

FIG. 3: Study of a two-band superconducting system in a square lattice with disorder in the l-channel with strength of disorder D=1.0. While (a),(b) and (c) studies the s, l PDOS and Total DOS respectively for the non-superconducting case (where intra and inter-band Hubbard potential U_s=U_l=U_{sl}=0.0) (d), (e) and (f) studies the effect of disorder on the corresponding superconducting system with only intra-band interaction.

has characteristic features of disordered DOS : namely increase in band-width and smoothing out of Van Hove singularities. The total DOS (Fig.3(c)), therefore, carries the signatures of disorder as well.

Next, we investigate the DOS of the same system considering only the intra-band Hubbard parameters to be non-zero i.e., $U_s = U_l = 4.0$ and $U_{sl} = 0.0$ (Fig.3(d),(e) and (f)). In this case only the intra-band pairing amplitudes Δ_s and Δ_l are non-zero (see Eqn(3)). We see that the s PDOS remains unaffected by randomness in the l-channel (comparing Fig.3(d) with Fig.1(b)), disorder however influences the l PDOS (comparing Fig.3(e) with Fig.1(b)). Since both the s PDOS and l PDOS are gapped, the total DOS remains gapped (Fig.3(f)). Similar behaviour also prevails with the inclusion of attractive inter-band interaction U_{sl}, provided the intraband pairing dominates *ie.* $U_{sl} < U_l$ and U_s.

The variation of the zero temperature superconducting order parameters Δ_s, Δ_l and Δ_{sl} are plotted as a function of the strength of disorder in Fig.4(a) where U_s=U_l=2.0 > U_{sl}=1.0. As expected for momentum independent pairing only the intra-band pairings are finite. Δ_s does not change as a function of disorder strength as it does not register the effect of the disorder in the l-channel. As the strength of disorder (D) is increased Δ_l reduces but remains finite even for D=3. Therefore in the chosen parameter regime for the two band system the situation is similar to that predicted by Anderson theorem[11] for single-band system, where the gap survives in the quasi-particle spectrum even in the presence of disorder.

Suhl *et al.*[6] using a generalized BCS Hamiltonian for the two band superconductor proposed a generalized expression for critical temperature T_c and temperature dependent pairing amplitude. As stated earlier, our two-band Hubbard Hamiltonian without the inter-band pairing term is identical to that of Suhl *et al.*. The expression for T_c for the s- and l-bands (T_c^s and T_c^l respectively) can be generalized to:

$$1 = |U_m| \int_{-\infty}^{\infty} dE \, \frac{\ll N_m(E) \gg}{2E} \tanh\left(\frac{E}{2k_B T_c^m}\right) \quad (20)$$

where, $m = s$ or l, while $\ll N_s(E) \gg$ and $\ll N_l(E) \gg$ are the s and l-band configuration averaged density of states in the normal state at energy E. Setting $U_s = U_l = 3.5$, U_{sl}=0 and $x = y = 0.5$ and keeping the system fixed at half-filling, we obtain the corresponding T_c^s and T_c^l for different values of D (see Fig.4(b)). As seen from this figure, T_c^s remains constant with increasing disorder strength D since randomness in the l-band does not affect the s-band in the presence of intra-band pairing alone. T_c^l is however suppressed with increasing D. At this point however it must be noted that only the higher of the two critical temperatures [T_c^s and T_c^l] is physically significant in this respect. So in the present case, T_c first decreases with disorder and then becomes constant when $T_c^s > T_c^l$.

These conclusions are further strengthened by a study of the pairing amplitude as a function of temperature, and the expressions for the temperature-dependent pairing amplitudes are :

$$1 = |U_m| \int_{-\infty}^{\infty} dE \frac{\ll N_m(E) \gg}{2\left(E^2 + \Delta_m^2\right)^{\frac{1}{2}}} \tanh\left(\frac{\left(E^2 + \Delta_m^2\right)^{\frac{1}{2}}}{2k_B T}\right)$$

for the $m = s$ or l-bands.

We see that with the increase in disorder strength D in the l-band the temperature dependent pairing amplitude Δ_l reduces much like the zero-temperature pairing amplitude (see Fig. 4(c)). Since randomness in the l-channel does not affect the s-band thus $\Delta_s(T)$ is not affected by D so we have plotted $\Delta_s(T)$ vs T only at D=0 (see Fig. 4(c)). We conclude from Fig. 4(b) and (c) that for temperatures below the critical temperatures though disorder (D) suppresses $\Delta(T)$, but does not reduce it to zero.

The next set of studies is the investigation of the increasing strength of the disorder D on a two band

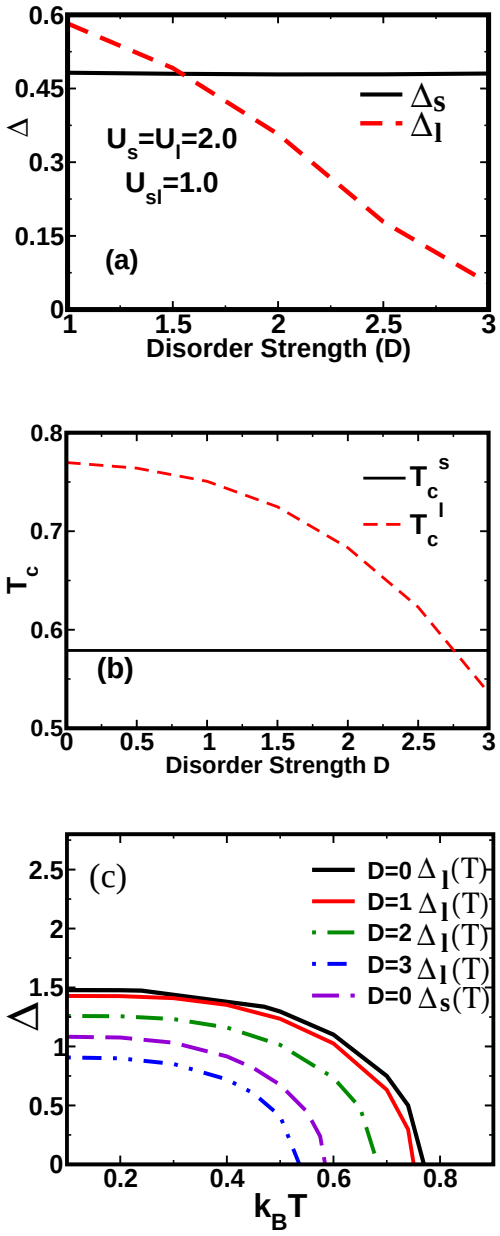

FIG. 4: (Color online) (a) Variation of Δ as a function of disorder strength (D) in the l-band when $U_s = U_l > U_{sl}$. (b) Variations of s-band and l-band critical temperatures T_c^s and T_c^l as a function of disorder strength D when only intra-band pairing occurs in a two-band s-wave superconductor in a square lattice. (c) Variation of Δ_s(T) and Δ_l(T) with T for various strengths of disorder D in the l-band.

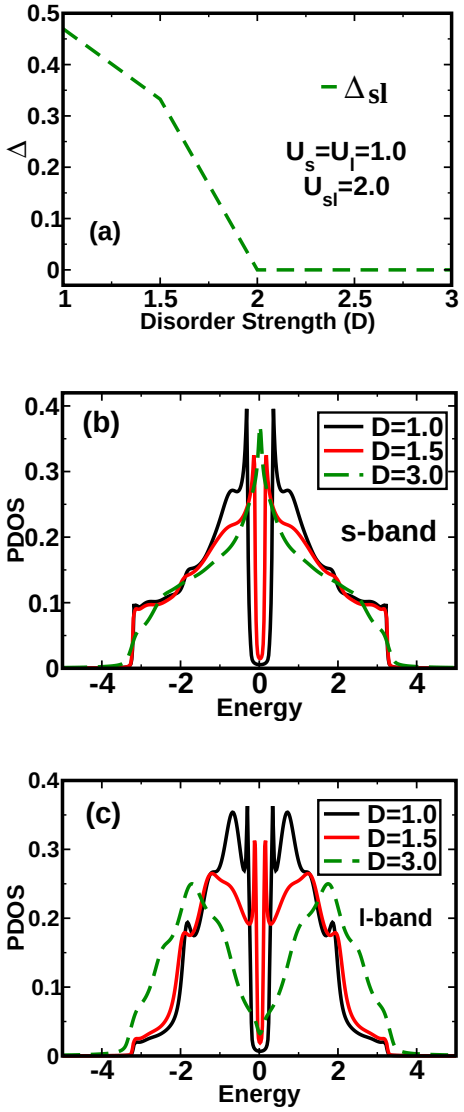

FIG. 5: (Color online) (a) Variation of Δ with disorder strength (D) in the l-band when U_s=U_l < U_{sl}.(b) and (c) studies DOS for a square-lattice superconducting system with disorder in the l-band when U_s= U_l < U_{sl}.

attractive-U Hubbard model with dominant inter-band attractive interaction $U_{sl} > U_s, U_l$. In the parameter regime U_s=U_l=1.0 < U_{sl} the dominant pairing is the inter-band pairing U_{sl} and it affects both the bands. In contrast to the case of only intra-band pairing , here for a critical strength of disorder D>2 the pairing amplitude Δ_{sl} vanishes indicating the possible disappearance of superconductivity [see Fig. 5(a)]. This is further illustrated in the DOS plot for the s and l channels in Fig. 5(b) and Fig. 5(c) respectively. Here the presence of randomness in the l channel affects Δ_{sl} and this in turn affects both s and l PDOS. With increasing disorder D in the l-channel the gaps both in the s PDOS and l PDOS reduces. Eventually finite DOS at the Fermi level is realized indicating absence of superconductivity.

Finally we address the situation when disorder is introduced in both s- and l-channels. When the interaction is such that $U_s = U_l > U_{sl}$ [Fig. 6(a)], then only Δ_s and Δ_l are non-zero even for strength of disorder as large as D=2.5 indicating the presence of superconductivity.

However in the limit $U_{sl} > U_s = U_l$ [Fig.6(b)], we see that Δ_{sl} decreases rapidly with disorder and finally vanishes. These features are very similar to the case when disorder was introduced in only one channel.

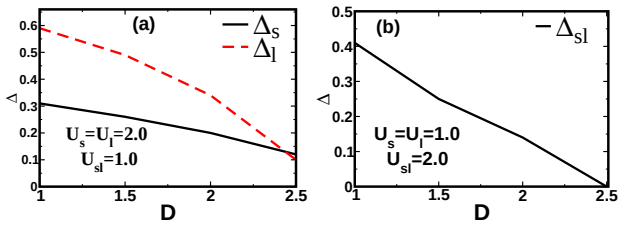

FIG. 6: A study of Δ as a function of disorder strength (D) in the s and l-band for (a) $U_s = U_l > U_{sl}$ and (b) $U_s = U_l < U_{sl}$ for a 2D superconducting system having two-bands. Here the intraband hopping integrals t_s=1.0 and t_l=0.5 and the interband hopping integral t_{sl}=0.0.

C. Summary.

In this paper we have developed a real space approach to study the effect of disorder on multi-band superconductivity using a two-band Hubbard Hamiltonian to model our system and augmented space vector-recursion[22,23] method to treat randomness in our system. We have established the accuracy of our method by comparing our results in ordered systems with those obtained earlier using other techniques. For ordered systems we have seen gaps in both bands in the presence of intraband pairing. In the presence of both intraband and interband momentum independent pairing, depending on the relative magnitude of the pairing strength, only a particular kind of pairing is possible for a half-filled $s-$like two band systems.

We have then studied the effect of randomness in one of the bands. When only intra-band pairing occurs, randomness in one channel does not affect the other. But in the presence of inter-band pairing both the bands are affected by randomness. By increasing the strength of disorder superconductivity survives in the presence of intra-band pairing although the pairing amplitudes decrease with disorder.However for interband pairing the gap in the quasiparticle spectrum ceases to exist beyond a critical value of the disorder strength. In the case of interband pairing, where the Cooper pairs are formed by electrons belonging to two different bands, we speculate that phase coherence of the superconducting state is more sensitive to disorder. The lack of phase coherence due to disorder is probably responsible for the disappearance of superconductivity. The same conclusion holds good when disorder is introduced in both the bands. Our calculation indicates inter-band pairing in multiband systems is not only interesting but opens up a paradigm beyond Anderson's theorem[11] to understand superconductivity in disordered systems.

Acknowledgment

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