Augmented space recursion study of the effect of disorder on superconductivity

Shreemoyee Ganguly,[1] A. Venkatasubramanian,[2] Kartick Tarafder,[1,2,*] Indra Dasgupta,[2,3] and Abhijit Mookerjee[4,†]
[1]*Department of Materials Science, S.N. Bose National Centre for Basic Sciences, JD-III Salt Lake City, Kolkata 700098, India*
[2]*Department of Physics, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India*
[3]*Department of Solid State Physics and Centre for Advanced Materials, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700 032, India*
[4]*Department of Materials Science and Advanced Materials Research Unit, S.N. Bose National Centre for Basic Sciences, JD-III Salt Lake City, Kolkata 700098, India*
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We present a real-space approach to study the effect of disorder on superconductivity. The method is based on augmented space formalism that goes beyond mean-field approximations for configuration averaging and effectively deals with the influence of configuration fluctuations of the neighborhood of an atom. In the regime of validity of Anderson's theorem our results for *s*- and *d*-wave dirty superconductors have excellent agreement with existing results. The formalism is extended and tested for random negative *U* Hubbard model. Having verified the reliability of our method we use it to study environment-dependent inhomogeneous randomness in disordered superconducting systems.

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I. INTRODUCTION

There has been considerable interest, during the last decade, in the study of the effects of disorder on superconducting properties of materials and inhomogeneous superconductors such as those enclosed by surfaces[1] or modified by magnetic fields. The Bogoliubov–de Gennes (BdG) formalism[2] provides a natural framework for a fully microscopic description of these phenomena. Unfortunately the BdG equations are difficult to solve as compared to simpler phenomenological approaches. In the recent times, however, there has been progress in the development of new methods of solution for the BdG equations both in real[3–13] and in reciprocal spaces.[14] There exists quite a large body of work where BdG equations have been solved in conjunction with the mean-field single-site coherent-potential approximation (CPA) (Refs. 15–17) in order to understand the physics of disordered superconductors. BdG equations have been solved in reciprocal space for realistic model Hamiltonians for the high-T_c cuprates.[18] They have also been solved using the real-space-based recursion method to study interface properties of *d*- and *s*-wave superconductors.[6] The real-space-based approach is attractive since lattice periodicity is not an *a priori* requirement. As a result a large variety of problems related to inhomogeneous superconductors may be treated. This has been illustrated in several recent works.[3–5,9,10,16,19–21]

The main aim of this paper is to present a real-space approach to study the effect of disorder on superconductivity going beyond standard mean-field techniques for the purpose of configuration averaging. This will be based on the augmented space recursion (ASR) formalism introduced by one of us.[22] 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 the analytic properties of the configuration-averaged Green's functions, which form an essential ingredient of the solution. Unlike single-site mean-field approximations, it can deal easily with off-diagonal disorder in real space. Such off-diagonal disorder arises as an essential part of disordered *d*-wave superconductivity. It also enables us to investigate the effect of inhomogeneous disorder such as clustering, segregation, and short-ranged order, all of which are beyond the scope of approaches such as the CPA and usually occur intrinsically in most disordered materials due to different chemical affinities of the constituents.

The effect of disorder on superconductivity is usually discussed in the framework of Anderson's theorem.[23] For *s*-wave superconductors, Anderson's theorem asserts that if the perturbation by disorder preserves the time-reversal invariance and the coherence length is long enough to guarantee that the pairing potential Δ does not fluctuate, then the absolute gap in the quasiparticle spectrum survives. The main effect of disorder is that the gap equation is modified where the density of normal state appearing in the gap equation is now replaced by its average over configurations. In contrast, for the case of superconductors whose Cooper pairs are of the exotic *p*-wave[24,25] or *d*-wave[16,19,21] character, even simple potential scattering that does not break time-reversal symmetry causes pair breaking. The above scenario, discussed in the framework of Anderson's theorem, is applicable only in the low disorder regime where the mean-free path is much larger than the Fermi wave vector. We shall apply our method to two situations: first a tight-binding negative *U* Hubbard model with on-site disorder only and next a random negative *U* Hubbard model where electrons attract each other provided that they are near certain randomly placed centers. In the second example, we shall address the issue of how many such centers are necessary to make the ground state superconducting. In this model the pairing potential will fluctuate and Anderson's theorem as described above may not be applicable. We shall examine our method in this limit. Having established our method in these two well-studied limits, we shall consider the physics of superconducting alloys with correlated disorder. Since the mean-field CPA techniques cannot deal with short-ranged or-

der, the advantage of the augmented space technique will become immediately evident.

The remainder of this paper will be organized as follows: in Sec. II we shall discuss our method. Section III will be devoted to test calculations, namely, ASR to disordered but nonsuperconducting systems (pairing potential $U=0$) and ordered BdG equations in square and cubic lattices, so that we may establish the accuracy of our basic technique. In Sec. IV we shall discuss superconducting alloys with on-site disorder. Random negative U Hubbard model will be discussed in Sec. V. Section VI will be devoted to superconducting alloys with correlated disorder followed by concluding remarks in Sec. VII. The Appendix will contain mathematical details of the vector-recursion technique.[26,27]

II. METHODOLOGY

To analyze the effect of disorder on a superconducting system we shall begin with the simplest model, namely, the single-band attractive Hubbard Hamiltonian in model lattices. The Hamiltonian is given by

$$\mathbf{H} = -t \sum_{\langle i,j\rangle,\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + \sum_{i\sigma} (\varepsilon_i - \mu_i) n_{i\sigma} - \sum_{\langle i,j\rangle,\sigma,\sigma'} |U_{ij}| n_{i\sigma} n_{j\sigma'}. \tag{1}$$

Here $\{c_{i\sigma}^{\dagger}, c_{i\sigma}\}$ are the usual electron-creation and electron-annihilation operators with spin σ on the site labeled as i of a square or a cubic lattice. The local charge-density operator is $n_i = n_{i\uparrow} + n_{i\downarrow}$, where $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$; μ is the chemical potential, t is the nearest-neighbor hopping amplitude, and ε_i is the local on-site energy at the site labeled as i. In this model, if $U_{ij} = -|U_{ii}|\delta_{ij}$ and $\sigma \neq \sigma'$, then the local attractive interaction gives rise to s-wave pairing. Whereas $U_{ij} = -|U_{ij}|(1-\delta_{ij})$, where j is a nearest neighbor of i on the lattice, the nonlocal attractive interaction gives rise to d-wave pairing.

The BdG mean-field decomposition[2] of the interaction terms give expectation values to the local and nonlocal pairing amplitudes,

$$\Delta_{ii} = -|U_{ii}|\langle c_{i\downarrow} c_{i\uparrow}\rangle, \quad \Delta_{ij} = -|U_{ij}|\langle c_{i\downarrow} c_{j\uparrow}\rangle, \tag{2}$$

and also to the local and nonlocal "densities,"

$$\langle n_{i\sigma}\rangle = \langle c_{i\sigma} c_{i\sigma}^{\dagger}\rangle \quad \langle n_{ij\sigma}\rangle = \langle c_{i\sigma} c_{j\sigma}^{\dagger}\rangle. \tag{3}$$

The effective quadratic BdG Hamiltonian becomes

$$\mathbf{H}_{\text{eff}} = -\sum_{i\neq j,\sigma} \hat{t} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i\sigma} (\varepsilon_i - \hat{\mu}_i) n_{i\sigma} + \cdots + \begin{cases} \sum_i (\Delta_{ii} c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} - \Delta_{ii}^{*} c_{i\uparrow} c_{i\downarrow}) & s\text{-wave pairing} \\ \sum_{i\neq j} (\Delta_{ij} c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} - \Delta_{ij}^{*} c_{i\uparrow} c_{j\downarrow}) & d\text{-wave pairing}, \end{cases} \tag{4}$$

where $\hat{\mu}_i = \mu - |U_{ii}|\langle n_i\rangle/2$ incorporates the site-dependent Hartree shift and $\hat{t} = t + |U_{ij}|\langle n_{ij}\rangle/2$ is the renormalized hopping integral. The extra feature of the Hamiltonian is that some of its terms are random. This effective Hamiltonian can be diagonalized by using the following transformation:

$$c_{i\uparrow} = \sum_n [\beta_{n\uparrow} u_n(r_i) - \beta_{n\downarrow}^{\dagger} v_n^{*}(r_i)],$$

$$c_{i\downarrow} = \sum_n [\beta_{n\downarrow} u_n(r_i) + \beta_{n\uparrow}^{\dagger} v_n^{*}(r_i)], \tag{5}$$

where β and $\beta^{\dagger}$ are quasiparticle operators and $u_n(r_i)$, $v_n(r_i)$ are the quasiparticle amplitudes associated with an eigen energy E_n.

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

$$\begin{pmatrix} H & \Delta \\ \Delta^{*} & -H^{\dagger} \end{pmatrix} \begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix} = E_n \begin{pmatrix} u_n(r_i) \\ v_n(r_i) \end{pmatrix}, \tag{6}$$

where (the excitation eigen value $E_n \geq 0$)

$$H u_n(r_i) = -\sum_j \left(t + \frac{1}{2}|U_{ij}|\langle n_{ij}\rangle \right) u_n(r_j) + (\epsilon_i - \hat{\mu}_i) u_n(r_i), \tag{7}$$

$$\Delta u_n(r_i) = \Delta_i u_n(r_i) + \Delta_{ij} u_n(r_j), \tag{8}$$

where j is the nearest neighbor of i. We can express the particle density $\langle n_i\rangle$ and the pairing potential in terms of the quasiparticle amplitude as

$$\langle n_i\rangle = 2\sum_n |u_n(r_i)|^2 f_n + |v_n(r_i)|^2 (1-f_n),$$

$$\Delta_i = |U_{ii}| \sum_n v_n^{*}(r_i) u_n(r_i) f_n - u_n(r_i) v_n^{*}(r_i)(1-f_n),$$

$$\langle n_{ij}\rangle = 2\sum_n u_n^{*}(r_i) u_n(r_j) f_n + v_n(r_i) v_n^{*}(r_j)(1-f_n),$$

$$\Delta_{ij} = |U_{ij}| \sum_n v_n^{*}(r_i) u_n(r_j) f_n - u_n(r_i) v_n^{*}(r_j)(1-f_n), \tag{9}$$

where f_n is the Fermi function. A fully self-consistent solution of Eq. (6) can be obtained provided both the normal potentials ($|U_{ii}|n_i$ and $|U_{ij}|n_{ij}$) and anomalous potentials (Δ_i and Δ_{ij}) are determined consistently with Eq. (9).

As mentioned earlier, since the Hamiltonian is random so all the physical quantities of interest [Eq. (9)] in such systems require to be configuration averaged. Earlier works had used the single-site CPA for this averaging. We shall turn to the ASR method introduced by Mookerjee[22] for this purpose.

The self-consistency criteria are set to 10^{-6} for the calculation of all self-consistent parameters throughout the present study. Clearly the normal Hartree-Fock term $|U_{ii}|\langle n_i\rangle/2$ is important as it gives rise to the position-dependent shift of the on-site energy. In our present case for the tight-binding lattice, we shall consider only the nearest-neighbor hopping interaction t. It is clear from the definition that if the coupling between the particle and hole space via the superconducting order parameter Δ is purely local (i.e., $U_{ij}=0$), then

the pairing potential will also be purely local (i.e., $\Delta_{ij}=0$) and when the interaction is nonlocal (i.e., $U_{ij}\neq 0$), then the nonlocal coupling between particle and hole space is present (i.e., $\Delta_{ij}\neq 0$).

The class of systems with which we shall begin our study will be substitutional binary disordered alloys with randomness in the diagonal site energies $\{\varepsilon_i\}$ only. We shall introduce site-occupation variables $\{n_i\}$ which take values 1 or 0 according to whether the site labeled as i is occupied by a A type or a B type of atom.

$$\varepsilon_i = \varepsilon_A n_i + \varepsilon_B(1-n_i), \tag{10}$$

where ε_A and ε_B are the possible on-site energies. We define the strength of disorder D as $|\varepsilon_A-\varepsilon_B|$.

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 (SRO), is given by

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

The "configuration space" of n_i, Φ_i, has rank 2 and is spanned by states $|A_i\rangle$ and $|B_i\rangle$.

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

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

where $|\varnothing_i\rangle=\sqrt{x}|A_i\rangle+\sqrt{y}|B_i\rangle$ is the "reference" state. 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 site i. The configuration states $|A_i\rangle$ and $|B_i\rangle$ are the eigenkets of $\tilde{N}_i$ corresponding to eigenvalues 1 and 0.

A representation of this operator in the basis is

$$\tilde{N}_i = x + (y-x)\gamma_i^\dagger\gamma_i + \sqrt{xy}(\gamma_i^\dagger+\gamma_i). \tag{11}$$

The operator $\gamma_i^\dagger$ creates a configuration fluctuation at site i about this reference state, e.g., $\gamma_i^\dagger|\varnothing_i\rangle=|1_i\rangle$. Since each site can have only two states, only *one* fluctuation is allowed per site. Thus γ_i are fermionlike operators: $\gamma_i^\dagger|1_i\rangle=0$ and $\gamma_i|\varnothing_i\rangle=0$. Thus,

$$\varepsilon_i = \varepsilon_B + \delta\varepsilon n_i$$

is replaced by

$$\langle\langle\varepsilon_i\rangle\rangle + (y-x)\delta\varepsilon\gamma_i^\dagger\gamma_i + \sqrt{xy}\delta\varepsilon(\gamma_i^\dagger+\gamma_i), \tag{12}$$

where $\delta\varepsilon=\varepsilon_A-\varepsilon_B$ and the degree of disorder $D=|\delta\varepsilon|$.

The augmented space theorem 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 $\Phi=\Pi^\otimes\Phi_i$,

$$\langle\langle\mathbf{A}(\{n_i\})\rangle\rangle = \langle\{\varnothing\}|\tilde{\mathbf{A}}\{\tilde{N}_i\}|\{\varnothing\}\rangle, \tag{13}$$

where $|\{\varnothing\}\rangle=\Pi_i^\otimes|\varnothing_i\rangle$ and $\tilde{\mathbf{A}}(\{\tilde{N}_i\})$ is the representation of the operator $\tilde{\mathbf{A}}$ in the configuration space Φ, constructed by replacing all random variables n_i by their corresponding operators $\tilde{N}_i$ and

$$\tilde{\mathbf{A}}(\{\tilde{N}_i\}) = \int\cdots\int \mathbf{A}(\{\lambda_i\})\prod d\mathbf{P}(\lambda_i). \tag{14}$$

$\mathbf{P}(\lambda_i)$ is the spectral density of the self-adjoint operator $\tilde{N}_i$. A compact way of representing a basis in configuration space is to denote it by the sequence of sites where we have a configuration fluctuation. This sequence is called the *cardinality sequence* and the meaning of the empty cardinality sequence $\{\varnothing\}$ then becomes obvious. For the present system the Hamiltonian contains the random variables $\{\varepsilon_i\}$. So we need to construct the Hamiltonian in the augmented space $\Psi=\mathcal{H}\otimes\Pi_i^\otimes\Phi_i$ by replacing all the random variables ε_i by the corresponding operators shown in Eq. (12). The effective augmented space Hamiltonian becomes

$$\begin{aligned}\tilde{\mathbf{H}}_{\mathrm{eff}} = &-\sum_{i\neq j,\sigma}\hat{t}c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma}(\langle\langle\varepsilon_i\rangle\rangle-\hat{\mu}_i)n_{i\sigma}\\ &+\sum_{i\neq j}(\Delta_{ij}c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - \Delta_{ij}^* c_{i\uparrow}c_{j\downarrow}) + \sum_i(\Delta_{ii}c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - \Delta_{ii}^* c_{i\uparrow}c_{i\downarrow})\cdots\\ &+\sum_{i\sigma}\delta\varepsilon n_{i\sigma}\{(y-x)\gamma_i^\dagger\gamma_i + \sqrt{xy}(\gamma_i^\dagger+\gamma_i)\}.\end{aligned} \tag{15}$$

Here all the symbols have the same meanings as before. We should note from Eqs. (2) and (3) that due to the coupling between parameters, the disorder in $\{\varepsilon_i\}$ is translated to the disorder in all the Hamiltonian parameters and the equations have to be solved self-consistently.

Basically the augmented space formalism maps a disordered Hamiltonian in the Hilbert space $\mathcal{H}$ onto an ordered "Hamiltonian" in the augmented space ($\Psi=\mathcal{H}\otimes\Phi$) which is constructed as the outer product of the space $\mathcal{H}$ and configuration space Φ of the random variables of the disordered Hamiltonian. The price that we pay for this mapping is that we now have to work in a much enlarged space. If $\mathcal{H}$ is of rank N then Φ has rank 2^N. Another way of looking at the Hamiltonian in the augmented space is that it is the collection of all possible Hamiltonians for all possible configurations of the system. After constructing the Hamiltonian in augmented space the augmented space theorem then automatically ensures that key entities such as the configuration-averaged diagonal-matrix element of the resolvent of the Hamiltonian is given by

$$\langle\langle\mathbf{G}(1,1,E)\rangle\rangle = \langle 1\otimes\varnothing|\tilde{\mathbf{G}}(E)|1\otimes\varnothing\rangle,$$

where $\tilde{\mathbf{G}}=(E\tilde{\mathbf{I}}-\tilde{\mathbf{H}}_{\mathrm{eff}})^{-1}$.

Haydock's recursion[28] method provides a recipe to calculate $\mathbf{G}(1,1,E)$. The same method when implemented in the augmented space[22] provides the configuration-averaged $\langle\langle\mathbf{G}(1,1,E)\rangle\rangle$. The physical quantities of interest [Eq. (9)] relevant to the study of superconductivity can be expressed as appropriate matrix elements of the Green's function (both diagonal as well as off diagonal, see the Appendix for details). We shall employ the vector-recursion technique introduced by Godin and Haydock[26,27] in augmented space to

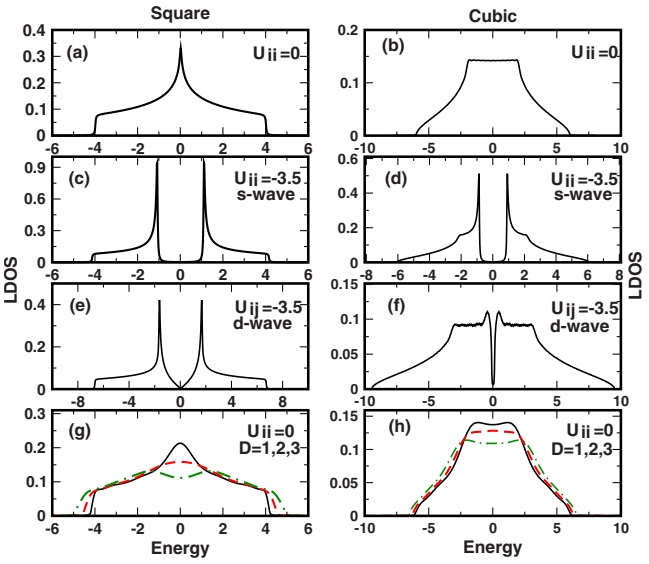

FIG. 1. (Color online) LDOS for the square (left column) and cubic (right column) lattices. In the first row, (a) and (b) are for nonrandom models $D=0$ with $\varepsilon_i=0$, $t=1$ and local Hubbard term $U_{ii}=0$. In the second and third rows (c)–(f) are for the same parameters except the local interaction $U_{ii}=-3.5a$. The order parameter Δ has *s*-like symmetry for (c) and (d) and *d*-like symmetry for (e) and (f). In the last row (g) and (h) have local interaction $U_{ii}=0$ but the diagonal term ε_i is random with disorder strengths $D=1$ (full curves), 2 (dashed curves), and 3 (dashed-dotted curves).

directly obtain the various configuration-averaged Green function. This has been described in some detail in the Appendix.

III. TEST CALCULATIONS ON ORDERED SUPERCONDUCTORS AND DISORDERED ALLOYS

We shall begin by carrying out calculations on test systems, where results are well known from other approaches. This is to establish the feasibility and numerical accuracy of our method. These test calculations are done on ordered superconductors and on disordered alloys in the absence of superconductivity.

The local density of states (LDOS) for the case when $U_{ii}=0$ for the ordered square and cubic lattices is shown on the top row of Fig. 1. The two LDOSs exactly match the standard calculations using the Bloch theorem. The square lattice LDOS has the band-center integrable Van Hove singularity and the two flanking kink singularities, while the cubic lattice LDOS is characterized by kink singularities at two ends of the constant LDOS at the band center. Both have square-root singularities at the band edges.

Since *s*-wave superconductivity is a local phenomenon we model the system by an attractive Hubbard Hamiltonian with $|U_{ij}|=0$ and $|U_{ii}|<0$ in Eq. (1). We take the local attractive interaction U_{ii} to be -3.5 and keep the system fixed at half filling. The BdG equations are solved recursively and self-consistently as described earlier. We have calculated 249 and 49 recursion steps exactly for the two-dimensional (2D) square and three-dimensional (3D) simple-cubic lattices, respectively, and then extrapolated to a further 2000 levels. After self-consistency in Δ_{ii} is achieved, the LDOS for the system is calculated by using the relation

$$\langle\langle n_1(E)\rangle\rangle = -\frac{1}{\pi}\lim_{\eta\to 0} \mathrm{Im}\, G^{++}(1,1,E+i\eta),$$

where + and − refer to electron and hole spaces of the BdG formalism.

The LDOSs for $U_{ii}=-3.5$ are shown in the second row of the same figure for the square and cubic lattices, respectively. As seen in Fig. 1 (second row), the LDOS has a central band gap with integrable infinite Van Hove singularities at the gap edges and the usual square-root singularities at the external band edges. The band gap is of course the signature of the nonvanishing zero-temperature local pairing amplitude ($\Delta_{ii}=1.09$ units for the square and 0.88 units for the cubic lattice). Δ_{ii} shrinks when we go from two to three dimensions. In an earlier work Martin and Annett[6] used the scalar-recursion method to solve the BdG equations. They kept Δ_{ii} fixed and changed $\langle n_i\rangle$ self-consistently. In contrast, in this work, the system is fixed at half filling. Thus their DOS, unlike ours, was not symmetric about the band gap.

We have also studied the completely nonlocal ($U_{ii}=0$) superconductivity for a nonrandom system. This type of superconductivity is generally associated with *d*-wave superconductors. To obtain the corresponding Hamiltonian, we consider $U_{ii}=0$ and $U_{ij}<0$ in Eq. (1). Also μ^* reduces to μ in this case. For nonlocal interaction, the order parameter has *d*-type symmetry, i.e., changes sign as we rotate by $\pi/2$ around a site. Vector recursion is carried out on the above Hamiltonian, for nonlocal attractive interaction $U_{ij}=-3.5$, until self-consistency is achieved for Δ_{ij} and $\langle n_{ij}\rangle$. The LDOS is calculated and shown in the third row of Fig. 1 for the square and cubic lattices. Here too the Van Hove singularities within the band and the square-root singularities at the external band edges are very prominent. The V-shaped opening that appears at the internal band edge is characteristic of *d*-wave superconductivity.[6,19] Also we observe that for this case the DOS that piles up at the gap edge is more smeared than for *s*-wave superconductivity and states are pushed to higher energies.

Finally, the last row of Fig. 1 shows the LDOS for the square and cubic lattices without any interaction, i.e., $U_{ii}=0$, $U_{ij}=0$ but with disorder in the diagonal term ε with disorder strengths $D=1$, 2, and 3 (concentration $x=0.5$). As expected the bandwidths increase with D and the Van Hove singularities are smoothed out. For the larger values of D a pseudogap begins to open up at the band center leading eventually to a split-band situation for very large values of D.

IV. SUPERCONDUCTING ALLOYS WITH DISORDER IN ON-SITE ENERGY

Our scheme for the study of a random binary substitutional alloy Hubbard model, with randomness only in the on-site energy, is similar to that for nonrandom systems. First we have studied the case of *s*-wave superconductivity where $|U_{ij}|$ is set to zero in the Hamiltonian and the local interaction

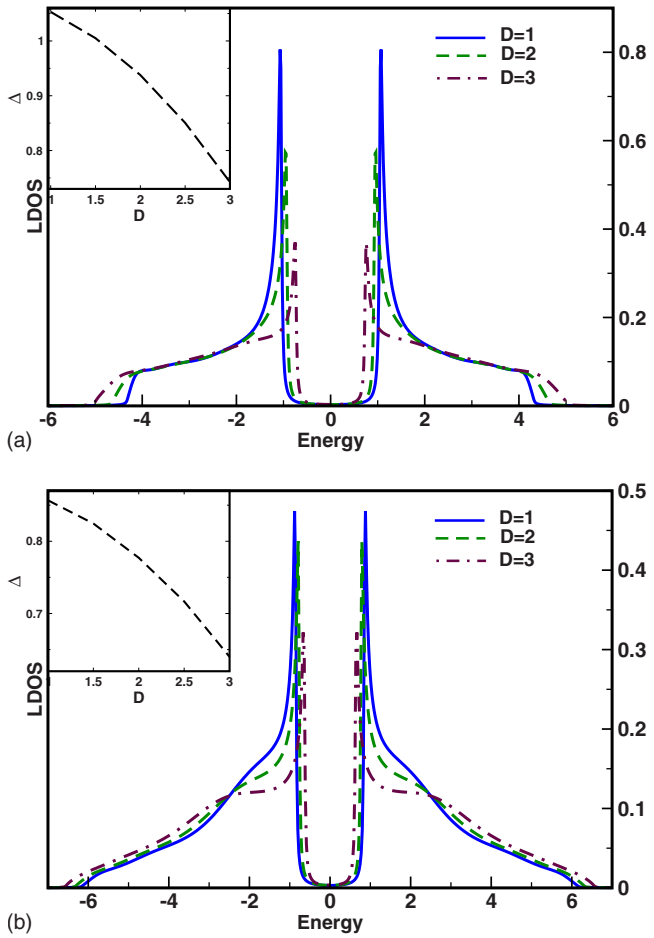

FIG. 2. (Color online) Local DOS for (a) square lattice and (b) cubic lattice with local interaction $U_{ii}=-3.5$. The system is homogeneously disordered with the strengths of disorder $D=1$, 2, and 3. The insets exhibit a variation in Δ with increasing D for the respective lattices.

U_{ii} is taken to be −3.5. We studied the half-filled 2D square lattice and 3D cubic lattice systems for different strengths of disorder D. The concentrations $x=0.5$ and $y=0.5$ were chosen in our calculations. The results of our calculation are displayed in Fig. 2. Our systems have homogeneous disorder with $D=1$, 2, and 3. With increasing disorder the LDOS that piles up at the internal gap edges decreases and states are pushed to higher energies. This observation was also made in a previous study[3] where randomness in the on-site energy was described by an independent continuous random variable V_i uniformly distributed over $[-V,V]$ at each site i. For both the square and cubic lattices we find that when the strength of disorder D is increased, superconductivity survives but the zero-temperature pairing amplitude reduces (see the inset of Fig. 2). This observation is supported by earlier studies.[1,3,4,15]

Having thus far kept the system fixed at half filling, we now investigate the behavior of zero-temperature pairing amplitude (Δ) as we vary the filling fraction from 0 (empty band) to 2 (fully occupied band). For square and cubic lattices, as seen in Fig. 3, Δ is maximum at half filling and decreases as we move away from half filling. The result of

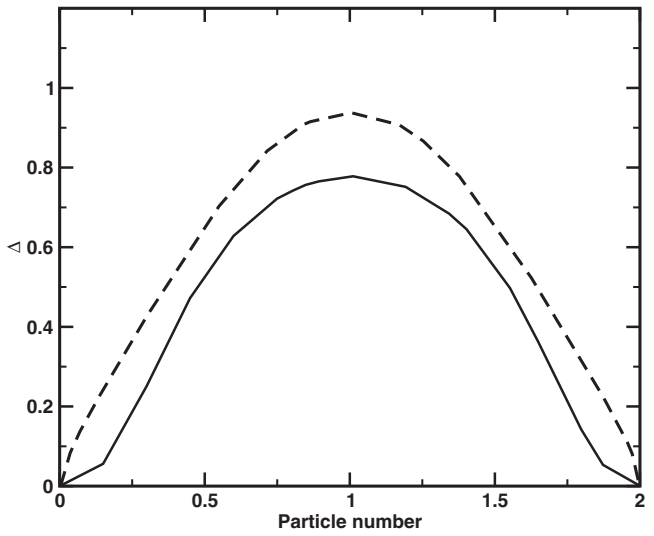

FIG. 3. Zero-temperature pairing amplitude (Δ) for (dashed line) square lattice and (solid line) a cubic lattice with $D=2$ as a function of filling fraction.

our calculation is similar to that obtained in CPA.[15] We gather from Fig. 3 that Δ is maximum for the particle-hole symmetric case when $n=1$ and $x=y=0.5$, as the order-parameter fluctuation vanishes in this regime and Anderson's theorem holds good irrespective of the strength of disorder. When the filling fraction (particle number) is either 0 or 2 then the coupling between the particle and hole space is not possible resulting in $\Delta=0$ as can be seen in Fig. 3.

We also studied the effect of disorder in ε_i on d-wave superconductivity. For this we set the local interaction potential $U_{ii}=0$ and the nonlocal interaction potential $U_{ij}\neq 0$. Now $\Delta_{ii}=0$ and $\mu_i^*=\mu_i$ in Eq. (4). The results that we get for the 2D case are in good agreement with earlier works.[16,19,29] As seen in Fig. 4 the behavior of d-wave superconducting systems under disorder is distinctly different from that of s-wave superconductors. Here strikingly the characteristic V-like dip that is the hallmark of nonrandom d-wave super-

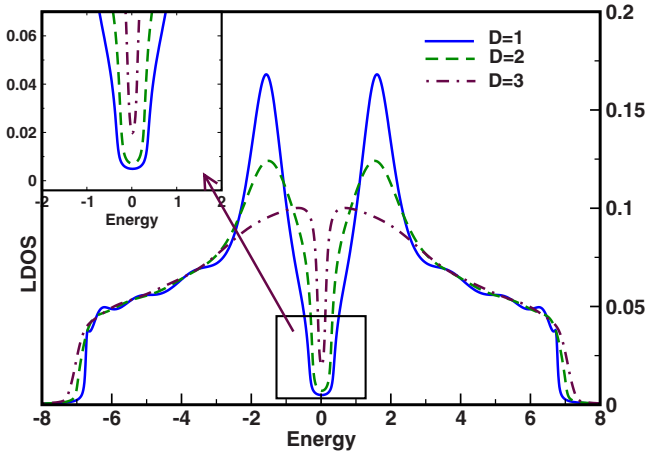

FIG. 4. (Color online) Local DOS for a 2D lattice with nonlocal interaction $U_{ij}=-3.5$. Here strength of disorder (D) is (a) 0 and (b) 1, 2, 3, and 4. The inset gives a closer view of the closing up of the V-like wedge in the DOS with increasing D.

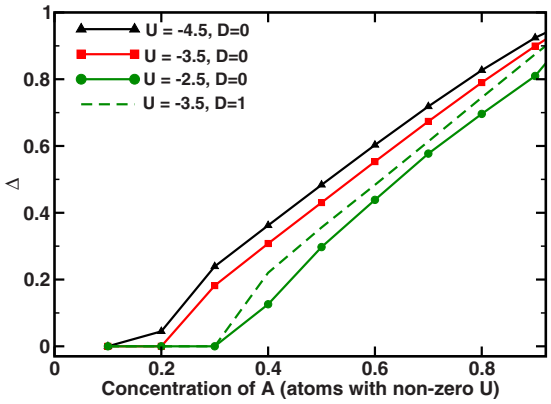

FIG. 5. (Color online) Zero-temperature pairing amplitude (Δ) for the square lattice with randomness in U_{ii} as a function of concentration of atoms with nonzero pairing potential. Only for the dashed curve disorder strength $D=1$.

conductivity (Fig. 4) closes up, i.e., the density of states becomes nonzero with the introduction of even the slightest of disorder. This is a signature of gapless superconductivity in contrast to the gapped one in the *s*-wave case.

V. RANDOM NEGATIVE *U* HUBBARD MODEL

In this section we shall consider the attractive Hubbard model with a random on-site interaction term where a fraction of the sites occupied by *A* type of atoms have finite pairing potentials $U_{ii}=U^A\neq 0$ while others occupied by *B* type of atoms have zero pairing potentials $U_{ii}=U^B=0$. For such a model we shall address the question whether there is a critical concentration x_0 of *A* atoms below which the system ceases to be superconducting.

The Hamiltonian under this condition in the augmented space is

$$\begin{aligned}\tilde{\mathbf{H}}_{\text{eff}} = &- \sum_{i\neq j,\sigma} t c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i\sigma} (\langle\langle \varepsilon_i \rangle\rangle - \mu) n_{i\sigma} \cdots + \sum_{i\sigma} (\delta\varepsilon_i - \delta\mu_i) \\ &\times \{(y-x)\gamma_i^{\dagger}\gamma_i + \cdots + \sqrt{xy}(\gamma_i^{\dagger} + \gamma_i)\} n_{i\sigma} \cdots \\ &+ \sum_i (\delta\Delta_{ii} c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} - \delta\Delta_{ii}^{*} c_{i\uparrow} c_{i\downarrow}) \{(y-x)\gamma_i^{\dagger}\gamma_i + \cdots \\ &+ \sqrt{xy}(\gamma_i^{\dagger} + \gamma_i)\}, \end{aligned} \tag{16}$$

where $\delta\varepsilon_i = \varepsilon^A - \varepsilon^B$, $\delta\mu_i = -|U^A|\langle n_i\rangle/2$, and $\delta\Delta_{ii} = -|U^A|\langle c_{i\downarrow} c_{i\uparrow}\rangle$. In the augmented space, we see the effect of randomness in U_{ii} in two terms: $\delta\mu_i$ which is diagonal in particle-hole space and $\delta\Delta_{ii}$ which is off diagonal in it.[30]

We carried out a systematic study of the behavior of zero-temperature pairing amplitude (Δ) as a function of concentration, x, of such negative U centers for different values of pairing potential (U_{ii}) to investigate the variation in the critical concentration below which the system ceases to be a superconductor.

As seen in Fig. 5, the critical concentration necessary for the system to be superconducting increases with the decreasing value of the attractive interaction U seen as a sharp drop in Δ in Fig. 5. In addition, for a given U with introduction of disorder in ε_i as well, the superconductivity is further suppressed and a larger concentration of *A* atoms with nonzero U value are necessary for the system to be superconducting. Such critical concentration was also determined through CPA calculations.[17]

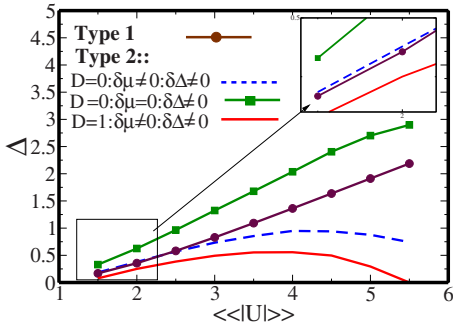

FIG. 6. (Color online) Study of pairing amplitude Δ as a function of average U. Here $\delta\mu$ is the diagonal term arising from disorder in U_{ii}. D and $\delta\Delta$ indicate disorder in ε_i and Δ_{ii}, respectively. The strength of disorder in ε_i is $D=1$, wherever present. The inset gives a closer view of the behavior of Δ_{ii} at low U_{ii}.

We also did a comparative study of two types of systems. The first type (type 1) is the one where all the sites of the system have the same pairing potential U (a uniform system) and the second (type 2) is where 50% of the sites have pairing potential $2U$ and others have pairing potential 0 (so that on the average $\langle\langle U\rangle\rangle$ is the same in both the systems). The results are illustrated in Fig. 6.

We see that when the strength of disorder (D) in ε_i is zero, and both diagonal and off-diagonal effects of disorder in U_{ii} ($D=0$, $\delta\mu$, and $\delta\Delta\neq 0$) are taken into account, the superconducting order parameter Δ is larger for type 2 in comparison to the uniform case (type 1), particularly for the small value of the interaction strength. This observation was also made by an earlier work done through Monte Carlo simulations[20] and is attributed to the proximity effects where a finite superconducting order parameter may be realized even on noninteracting sites due to the tunneling of the Cooper pairs from the interacting sites. This effect is particularly important at weak coupling (small U or Δ) where the coherence length $\xi = \frac{\hbar v_f}{\pi\Delta}$ is large.

Next we have gone further and investigated the role of the particular terms in Hamiltonian (16) that produces this behavior. To do this (as seen in Fig. 6) we first studied the sole effect of the term, off diagonal in electron-hole space, arising from randomness in U_{ii} on the system ($D=0$, $\delta\mu=0$ but $\delta\Delta\neq 0$). This term causes Δ to increase with an increase in U_{ii} and is particularly prominent for small values of U. This is because at lower U_{ii} the coherence length is longer; thus tunneling of Cooper pairs from interacting to noninteracting sites is possible as we have argued earlier. On the other hand, the term diagonal in electron-hole space, arising from this randomness ($\delta\mu$), plays a role much similar to $\delta\varepsilon_i$ in reducing Δ. So it is the competition between the terms diagonal and off diagonal in electron-hole space that arise from randomness in U_{ii} ($\delta\mu$ and $\delta\Delta$, respectively) which determines the behavior of Δ. Since at lower U_{ii} tunneling of Cooper pairs is facilitated, thus, in this region the effect of the off-

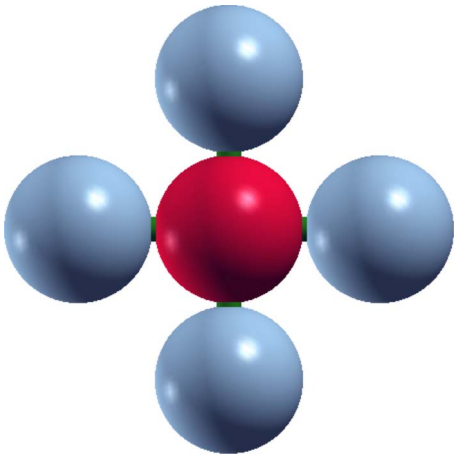

FIG. 7. (Color online) An central atom at a site 0 of a square lattice associated with its four nearest neighbors at 1–4

diagonal term ($\delta\Delta$) in enhancing Δ is more dominant. For nonzero on-site disorder D ($D=1$), the superconducting order parameter Δ is further suppressed.

VI. SUPERCONDUCTING ALLOYS WITH CORRELATED DISORDER

Instead of homogeneous disorder if there are short-ranged configuration correlations in the system, then the single-site CPA is unable to describe the situation adequately. We can use the generalized augmented space method introduced by Mookerjee and Prasad.[31] The method has been described in great detail in Ref. 31 and here we shall introduce only those essential ideas which are necessary for our exposition.

To start with, let us assume that SRO extends up to the first nearest neighbor only. For a square lattice the nearest-neighbor cluster is shown in Fig. 7. Let us consider a site labeled 0 (shown as a dark sphere) and the occupation variable associated with this site n_0.

The occupation variables associated with its four nearest neighbors n_k ($k=1,\ldots,4$) are correlated with n_0 but not with one another. Further none of the other occupation variables associated with more distant sites are correlated with n_0. We may then write the joint probability density as

$$P(\{n_m\}) = P(n_0)\prod_{k=1}^{4} P(n_k|n_0)\prod_{m>4} P(n_m).$$

The generalized augmented space theorem also associates with the random variable n_k a corresponding operator $\tilde{N}_k$ in augmented space. The construction of that operator has been discussed in detail in the earlier paper.[31] We can characterize short-ranged order by a Warren-Cowley parameter $\alpha(R)=1-P_{AB}(R)/x$, where x is the concentration of an A type of atom and $P_{AB}(R)$ is the probability of finding a B atom at a distance R from an A atom. Using this α, the conditional probabilities are given by the following.

For $k=0$ and $k>4$

$$P(n_k) = x\delta(n_k-1) + y\,\delta(n_k). \tag{17}$$

For $1\le k\le 4$

$$P(n_k|n_0=1) = (x+\alpha y)\delta(n_k-1) + (1-\alpha)y\,\delta(n_k),$$

$$P(n_k|n_0=0) = (1-\alpha)x\delta(n_k-1) + (y+\alpha x)\delta(n_k). \tag{18}$$

We note that when $\alpha=0$ there is no SRO in the system and the conditional probabilities for n_k when $1\le k\le 4$ reduces to the unrestricted probability for n_k when $k=0$ and $k>4$. While $\alpha<0$ indicates a tendency toward ordering, $\alpha>0$ indicates a tendency toward phase segregation.

In the full augmented space, the operators which replace the occupation variables are the same as Eq. (11) for site 0 and its far environment. However, for its nearest neighbors $k=1-4$,

$$\begin{aligned}\tilde{N}_k = {} & x + (y-x)\gamma_k^\dagger\gamma_k + \alpha(y-x)\gamma_0^\dagger\gamma_0 - 2\alpha(y-x)\gamma_k^\dagger\gamma_k\gamma_0^\dagger\gamma_0 \\ & + B_1(\gamma_k+\gamma_k^\dagger) + B_3(\gamma_0+\gamma_0^\dagger)\cdots + (B_2-B_1)\gamma_0^\dagger\gamma_0(\gamma_k+\gamma_k^\dagger) \\ & + (B_4-B_3)\gamma_k^\dagger\gamma_k(\gamma_0+\gamma_0^\dagger) + B_5(\gamma_k+\gamma_k^\dagger)(\gamma_0+\gamma_0^\dagger),\end{aligned} \tag{19}$$

where

$$B_1 = x\sqrt{(1-\alpha)y(x+\alpha y)} + y\sqrt{(1-\alpha)x(y+\alpha x)},$$

$$B_2 = y\sqrt{(1-\alpha)y(x+\alpha y)} + x\sqrt{(1-\alpha)x(y+\alpha x)},$$

$$B_3 = \alpha\sqrt{xy} = -B_4,$$

$$B_5 = \sqrt{xy}[\sqrt{(1-\alpha)y(x+\alpha y)} - \sqrt{(1-\alpha)x(y+\alpha x)}].$$

We note that as $\alpha\to 0$ the above equation is reduced to Eq. (11).

We now follow the augmented space theorem and replace all the occupation variables $\{n_m\}$ by their corresponding operators. The configuration average is the specific matrix element between the *reference* state $|\{\varnothing\}\rangle$ as discussed earlier. We also note that the choice of the *central* site labeled as 0 is immaterial. If we translate this site to any other and apply the lattice translation to all the sites, the Hamiltonian in the full augmented space remains unchanged. This formulation of SRO also possesses lattice translational symmetry, provided that the short-range order is homogeneous in space, as we consider it to be in our present study.

Figure 8 shows the results of the ASR calculations. We see that for disorder in ε_i alone, the zero-temperature gap is minimum when α is negative, i.e., the system has an ordering tendency and maximum when α is positive, i.e., the system tends to phase segregate. For perfect homogeneous disorder ($\alpha=0$), the situation is in between. Thus binary substitutional alloys with phase segregating tendency tends to support superconductivity better than alloys which tend to order.

Next we investigate the behavior of a system with random U_{ii} where *only* the term off diagonal in electron-hole space, arising from the disorder in U_{ii}, is considered. When we introduce short-ranged order in the system we observe the effect of randomness in U_{ii} to be quite different from randomness in ε_i. For randomness in U_{ii}, ordering supports superconductivity as can be seen in Table I. This is because ordering favors tunneling of Cooper pairs from the interacting to the noninteracting sites (now the noninteracting and

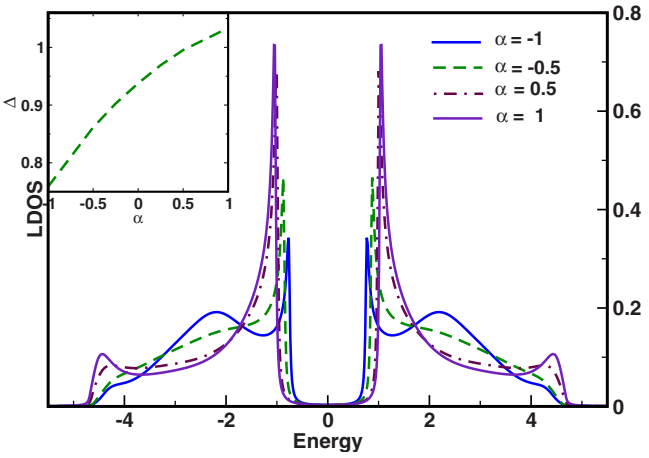

FIG. 8. (Color online) Local DOS for a 2D lattice with local interaction $U_{ii}=-3.5$, the strength of disorder $D=2$, and the short-range order parameter $\alpha=-1$, -0.5, 0, 0.5, and 1. The inset exhibits a variation of Δ with α.

interacting sites are near neighbors of each other). Thus even the noninteracting sites develop a finite value of Δ_{ii}, resulting in a larger value of the zero-temperature pairing amplitude as compared to phase segregation. When we have randomness in both U_{ii} and ε_i, the competition between the two effects sets in, and for large disorder strength (D) the onsite disorder overwhelms the randomness in U_{ii} and we find that phase segregation is more effective for the realization of superconductivity (see Table I, third row).

VII. SUMMARY

In this paper, we have proposed the augmented space vector-recursion method as a very effective real-space approach to study the effect of disorder on superconductivity beyond the mean-field approximation. We have established the accuracy of our method by comparing its results with those obtained by other techniques, for both s- and d-wave superconductors. We have seen that while for s-wave superconductors the gap in the quasiparticle spectrum survives even in the presence of disorder (the system is in the limit of validity of Anderson's theorem), for the exotic d-wave case it vanishes in the presence of slightest disorder. In addition, considering a system where electrons attract each other provided that they are near certain centers, we see that a critical number of such centers are necessary for superconductivity to survive in the system. Our results using the ASR method are in excellent agreement with that available in the literature.

TABLE I. Behavior of zero-temperature pairing amplitude for randomness in U_{ii} and ε_i.

$\langle\langle\lvert U\rvert\rangle\rangle$ Square lattice	D	$\Delta(\alpha=-1)$	$\Delta(\alpha=0)$	$\Delta(\alpha=1)$
1.75	0.0	0.490	0.470	0.460
1.75	0.3	0.470	0.463	0.457
1.75	1.5	0.210	0.320	0.380

Satisfied about the reliability of our method, we use it to study the effect of environment-dependent randomness of various terms of the Hamiltonian. This would not have been possible using any single-site mean-field approximations such as the CPA. For correlated disorder in ε_i segregation tendency supports superconductivity while for a system where only some sites are interacting, ordering facilitates tunneling of Cooper pairs from interacting to noninteracting sites and thus favors superconductivity. However for a higher value of the effective-pair interaction potential U the coherence length falls off and such tunneling of Cooper pairs becomes difficult.

The advantage as well as the strength of the recursion method is that it can easily be generalized to many band Hubbard models, models with off-diagonal disorder, and even in complex lattices. Coupled with first-principles techniques such as the tight-binding linear muffin-tin orbital method, we can establish a methodology for the study of realistic materials. We intend to extend our methodology to study various interesting aspects of superconductivity in real disordered materials in the future.

APPENDIX: THE VECTOR-RECURSION METHOD

We shall describe the solution of Eq. (6) self-consistently with Eq. (9) in some details. In this case we shall use the vector-recursion method by Haydock and Godin.[26,27] Using this method we can calculate the Green's function for the system which is given by (considering local interaction alone)

$$\mathbf{G}(E) = (E\mathbf{I} - \mathbf{H})^{-1}. \tag{A1}$$

Here the bold operators are 2×2 operators in a space spanned by "electron" (labeled by +) and "hole" excitations (labeled by −),

$$\mathbf{I} = \begin{pmatrix} I & O \\ O & I \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} H & \Delta \\ \Delta^* & -H^\dagger \end{pmatrix}.$$

The basis elements are labeled by the site index i and the electron-hole index α (=+ or −), $\{\Phi_{i\alpha}\}$.

The vector recursion is essentially a change in basis $\{\Phi_{i\alpha}\} \Rightarrow \{\mathbf{V}^{(n)}\}$ with $n=1,2,\ldots$, in which the Hamiltonian assumes a block tridiagonal form. We begin by choosing

$$\mathbf{V}^{(1)} = (\Phi_{1+} \quad \Phi_{1-}) = (V_+^{(1)} \quad V_-^{(1)}),$$

each member of the row are themselves $2N$-dimensional columns (N is the number of sites i).

The subsequent basis members are generated recursively from the three-term recursion relation suggested by Godin and Haydock,

$$\mathbf{H}\mathbf{V}^{(n)} = \mathbf{V}^{(n-1)}\mathbf{B}_n^\dagger + \mathbf{V}^{(n)}\mathbf{A}_n + \mathbf{V}^{(n+1)}\mathbf{B}_{n+1}, \tag{A2}$$

where $\mathbf{A}_n$, $\mathbf{B}_{n-1}$ are 2×2 matrices.

The recurrence relation (A2) gives $\mathbf{A}_n$ from the condition of orthogonality of $\mathbf{V}^{(n)}$ to $\mathbf{V}^{(n+1)}$,

$$\mathbf{A}_n = \{[\mathbf{V}^{(n)}]^\dagger \odot \mathbf{V}^{(n)}\}^{-1}\{[\mathbf{V}^{(n)}]^\dagger \odot \mathbf{H}\mathbf{V}^{(n)}\}. \quad \text{(A3)}$$

To calculate $\mathbf{B}^{(n+1)}$ we use the condition of orthogonality of the two columns of $\mathbf{V}^{(n+1)}$. In order to impose this condition we consider

$$\mathbf{W}^{(n)} = \mathbf{H}\mathbf{V}^{(n)} - \mathbf{V}^{(n)}\mathbf{A}_n - \mathbf{V}^{(n-1)}\mathbf{B}_n^\dagger. \quad \text{(A4)}$$

We construct two $(2N)$ column vectors ξ_+ and ξ_- from the two rows of $\mathbf{W}^{(n)}$ and then set about to Gram-Schmidt orthonormalizing this set,

$$\xi_+ = V_+^{(n+1)} b_{11} \Rightarrow b_{11} = (\xi_+^\dagger \xi_+)^{1/2}, \quad \text{(A5)}$$

$$\xi_- = V_+^{(n+1)} b_{12} + V_-^{(n+1)} b_{22},$$

$$\Rightarrow b_{12} = V_+^{(n+1)} \xi_-: \quad b_{22}^2 = \xi_-^\dagger \xi_- - b_{12}^2. \quad \text{(A6)}$$

By comparing Eqs. (A2) and (A4) it is evident that

$$\mathbf{B}_{n+1} = \begin{pmatrix} b_{11} & 0 \\ b_{12} & b_{22} \end{pmatrix}.$$

Thus initially knowing $\mathbf{V}^{(1)}$ we can calculate $\mathbf{A}_1$ from Eq. (A3). Then we can construct $\mathbf{W}^{(1)}$ [Eq. (A4)] ($\mathbf{B}_1$ is taken to be zero). Knowing $\mathbf{W}^{(1)}$ (thus corresponding ξ_+ and ξ_-) the different components of $\mathbf{B}_2$ can be obtained by the Gram-Schmidt orthonormalization procedure described above. Then the two columns of $\mathbf{V}^{(2)}$ can be calculated from Eqs. (A5) and (A6) and the procedure repeated resulting in the calculation of $\mathbf{A}_2$ and $\mathbf{B}_3$ and so on recursively. $\mathbf{V}^{(n)}$ represents a basis for solution of the Schrödinger equation in regions increasingly remote from initial state with increase in n, yielding the coefficients $\mathbf{A}_n$ and $\mathbf{B}_n$ which are in turn less and less significant in determining the local density of states with increasing n.

After performing the above recursion we can write the representation of the Green's operator as

$$(E\mathbf{I} - \mathbf{H})^{-1} = \begin{pmatrix} E\mathbf{I} - \mathbf{A}_1 & -\mathbf{B}_2 & 0 & 0 & \cdots \\ -\mathbf{B}_2^\dagger & E\mathbf{I} - \mathbf{A}_2 & -\mathbf{B}_3 & 0 & \cdots \\ 0 & -\mathbf{B}_3^\dagger & E\mathbf{I} - \mathbf{A}_3 & -\mathbf{B}_4 & \cdots \\ 0 & 0 & -\mathbf{B}_4^\dagger & \ddots & \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}^{-1}, \quad \text{(A7)}$$

where the elements are zero apart from the diagonal and just upper and lower diagonal positions. The (11) element of the Green's operator (A7) can be calculated by repeated applications of the partition theorem or downfolding,

$$\mathbf{G}(1,1,E) = (E\mathbf{I} - \mathbf{A}_1 - \mathbf{B}_2^\dagger \mathbf{G}^{(1)} \mathbf{B}_2)^{-1},$$

$$\mathbf{G}^{(1)} = (E\mathbf{I} - \mathbf{A}_2 - \mathbf{B}_3^\dagger \mathbf{G}^{(2)} \mathbf{B}_3)^{-P_1},$$

$$\mathbf{G}^{(n)} = (E\mathbf{I} - \mathbf{A}_{n+1} - \mathbf{B}_{n+2}^\dagger \mathbf{G}^{(n+1)} \mathbf{B}_{n+2})^{-P_n},$$

$$n = 1,2,\ldots, \quad \text{(A8)}$$

where $\mathbf{O}^{-P_n}$ is an inverse of the operator $\mathbf{O}$ in the subspace spanned by $\{\mathbf{V}^{(n+1)}, \mathbf{V}^{(n+2)}, \ldots\}$.

In principle this matrix continued fraction is infinite in length, but as we mentioned earlier that for the local-density-of-state calculation the coefficient matrices are less and less significant with increasing recursion steps and tend to converge. So in practice we can end it with a *terminator* function or go up to a very large number of steps by extrapolating the coefficients and then terminating it by a zero matrix, giving the energy a very small imaginary part. In this work we have used the second technique.

Now, the elements of the matrix Green's function has rank 2,

$$\mathbf{G}(1,1,E) = \begin{pmatrix} G^{++}(1,1,E) & G^{+-}(1,1,E) \\ G^{-+}(1,1,E) & G^{--}(1,1,E) \end{pmatrix}. \quad \text{(A9)}$$

The advantage of this method over the scalar-recursion method used by Martin and Annett[6] is that in this method we get all the elements of the Green's function matrix [Eq. (A9)] at one go. The price that we pay for it is that we now have to work with larger basis sets.

So from the expression of the Green's function we can easily calculate the local density of states by using the relation

$$n_1(E) = -\frac{1}{\pi}\lim_{\eta\to 0} \mathrm{Im}\, G^{++}(1,1,E+i\eta). \quad \text{(A10)}$$

η is an infinitesimal positive imaginary part of the energy. For calculating the density of states from the matrix continued fraction representation of the Green's function, we need to give a finite value to η so that the Green's function is calculated away from the pole in the real axis. The small η gives a small Lorentzian broadening to the contribution of each pole and the DOS will appear smooth if it is much larger than the separation of the poles of the Green's function.

We can also express the particle density and the pair interaction potential and related terms off diagonal in real space (in case $U_{ij} \neq 0$) in terms of the Green's function as

$$\langle n_1 \rangle = -\frac{1}{\pi}\lim_{\eta\to 0} \mathrm{Im} \int_{-\infty}^{\infty} [\mathbf{G}^{++}(1,1,E+i\eta) f_n + \mathbf{G}^{--}(1,1,E+i\eta) \times (1-f_n)] dE,$$

$$\Delta_{11} = -\frac{1}{\pi}\lim_{\eta\to 0} \mathrm{Im} \int_{-E_c}^{+E_c} [\mathbf{G}^{+-}(1,1,E+i\eta) f_n + \mathbf{G}^{-+}(1,1,E+i\eta) \times (1-f_n)] dE,$$

$$\langle n_{12} \rangle = -\frac{1}{\pi}\lim_{\eta\to 0} \mathrm{Im} \int_{\infty}^{\infty} [\mathbf{G}^{++}(1,2,E+i\eta) f_n + \mathbf{G}^{--}(1,2,E+i\eta) \times (1-f_n)] dE,$$

$$\Delta_{12} = -\frac{1}{\pi}\lim_{\eta\to 0} \mathrm{Im} \int_{-E_c}^{+E_c} [\mathbf{G}^{+-}(1,2,E+i\eta) f_n + \mathbf{G}^{-+}(1,2,E) \times (1-f_n)] dE, \quad \text{(A11)}$$

where the energy interval $[-E_c,+E_c]$ is the short interval around the Fermi energy of the system where the interaction has effect. In order to obtain the off-diagonal elements $G^{\alpha\alpha'}(1,2,E)$, we need to start the recursion with the initial basis matrix $\mathbf{V}^{(1)}=(V_+^{(1)}\ V_-^{(1)})$, where $V_\alpha^{(1)}=[\Phi_{1\alpha}+\Phi_{2\alpha}]/\sqrt{2}$. The continued fraction analysis then gives function $\mathbf{G}_{\text{nonlocal}}$ as

$$\mathbf{G}_{\text{nonlocal}}=\begin{pmatrix} G^{++}(1,1,E)+G^{++}(1,2,E) & G^{+-}(1,1,E)+G^{+-}(1,2,E) \\ G^{-+}(1,1,E)+G^{-+}(1,2,E) & G^{--}(1,1,E)+G^{--}(1,2,E) \end{pmatrix}=\mathbf{G}(1,1,E)+\mathbf{G}(1,2,E). \tag{A12}$$

Then we may obtain the required elements to calculate the expressions in Eq. (A11) using $\mathbf{G}_{\text{nonlocal}}$ [Eq. (A12)] and $\mathbf{G}(1,1,E)$ [Eq. (A9)].

*Also at Department of Physics and Materials Science, Materials Theory Division, Ångstronlaboratoriet, Lägerhyddsv. 1, Box 530, 75121 Uppsala, Sweden.

†abhijit@bose.res.in

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