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Korringa-Kohn-Rostoker nonlocal coherent-potential approximation

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We introduce the Korringa-Kohn-Rostocker nonlocal coherent-potential approximation (KKR-NLCPA) for describing the electronic structure of disordered systems. The KKR-NLCPA systematically provides a hierarchy of improvements upon the widely used KKR-CPA approach and includes nonlocal correlations in the disorder configurations by means of a self-consistently embedded cluster. The KKR-NLCPA method satisfies all of the requirements for a successful cluster generalization of the KKR-CPA; it remains fully causal, becomes exact in the limit of large cluster sizes, reduces to the KKR-CPA for a single-site cluster, is straightforward to implement numerically, and enables the effects of short-range order upon the electronic structure to be investigated. In particular, it is suitable for combination with electronic density-functional theory to give an *ab initio* description of disordered systems. Future applications to charge correlation and lattice displacement effects in alloys, and spin fluctuations in magnets amongst others, are very promising. We illustrate the method by application to a simple one-dimensional model.

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I. INTRODUCTION

Over the past 30 years or so, the coherent-potential approximation[1] (CPA) has proved to be a generally reliable method for dealing with disordered systems.[2,3] However, being in essence a single-site mean-field theory,[4] the CPA fails to take into account the effect of nonlocal potential correlations due to the disorder in the environment of each site, and hence leaves much important physics out of consideration. Consequently, considerable effort has been spent in trying to find a way of improving it systematically by a multisite or cluster generalization. Surprisingly, this has turned out to a very difficult problem,[5] and a viable solution has been proposed only recently. The new method has emerged from the dynamical cluster approximation[6–8] (DCA) which was directed originally at describing dynamical spin and charge fluctuations in simple Hubbard models of strongly correlated electron systems. Recently, its static limit has been adapted by Jarrell and Krishnamurthy for a simple tight-binding model of electrons moving in a disordered potential.[9] The same problem was investigated by Moradian *et al.*[10] In this paper we develop the ideas behind this approximation further, and demonstrate how they can be combined with realistic, *ab initio* descriptions of systems of interacting electrons in disordered systems.

Since the language of our multiple-scattering theory is so different from that of the context in which the DCA is usually deployed, we therefore elaborate on this relationship. First, we note that the DCA was formulated to describe short-range correlations within the framework of the dynamical mean field theory[11] (DMFT) of spin and charge fluctuations in many-electron systems. Second, we recall that the DMFT can be regarded as the dynamical generalization of the CPA for the Hubbard ‘‘alloy analogy’’ problem.[12,13] Thus, in the light of these remarks, it is natural to investigate the static version of the DCA as a generalization of the CPA, which includes a description of short-range order. Indeed, Jarrell and Krishnamurthy[9] already studied the problem of electronic structure in random alloys from this point of view. In this paper we tackle the same problem using an identical conceptual framework but a very different description of the electrons afforded by multiple-scattering theory.[14,15] To make the above remarks more specific, we would like to highlight two of the principal differences between our treatment of the problem and that of Ref. 9. First, we do not make use of a tight-binding model Hamiltonian but numerically solve a Schrödinger equation in each unit cell and match the ‘‘outgoing wave’’ solution to the incoming waves from all the other unit cells. This is known as the multiple-scattering approach[14,15] to the problem of electronic structure in solids and is the foundation of the Korringa-Kohn-Rostoker (KKR) band theory method. Consequently, the principal virtue of our formalism, as opposed to those based on tight-binding model Hamiltonians is that it prepares the ground for first-principles calculations based on density-functional theories.[16] The second difference is a formal consequence of the first. In multiple-scattering theories the object of interest is not the self-energy, and the diagrammatic language of perturbation theory is not used. We will show that the quantities that play the role of the self-energy in multiple-scattering theory are the effective scattering amplitudes $\underline{\hat{t}}$ and effective structure constants $\underline{\widehat{G}}(\mathbf{R}^{ij})$, which are also the natural concepts in effective-medium theories.[17] In short, these formal reasons fully account for the fact that we do not base our arguments on ‘‘restoring momentum conservation’’ and introducing approximate Laue functions to renormalize diagrams, but we construct our theory in terms of real- and reciprocal-space clusters. Nevertheless, we believe that our final algorithm described in Sec. II E is equivalent to those investigated by Jarrell and Krishnamurthy.[9] Our aim in reformulating the problem is to facilitate the deployment of the method as a first-principles calculation, in other words to develop a nonlocal (NL) KKR-CPA.[18]

In brief, our KKR-NLCPA method introduces effective structure constants, and this enables us to define an effective medium that includes nonlocal potential correlations over all length scales. Using a ‘‘coarse-graining’’ procedure inspired by the DCA, we can then derive a self-consistent ‘‘cluster generalization’’ of the KKR-CPA,[18] which determines an approximation to this effective medium by including nonlocal correlations up to the range of the cluster size. The KKR-NLCPA satisfies all of the requirements for a successful cluster generalization of the KKR-CPA as listed by Gonis.[5] In particular, the KKR-NLCPA becomes exact in the limit of large cluster sizes where it includes nonlocal correlations over all length scales, and recovers the KKR-CPA for a single-site cluster. The method is fully causal, allows the effects of short-range order to be modeled, and can be implemented numerically for realistic systems.

The outline of this paper is as follows. In the following section we describe the formalism for the KKR-NLCPA. We explain our KKR-NLCPA algorithm and show how to include short-range order. We describe in more detail how to carry out the coarse graining with reference to simple cubic, body-centered-cubic, and face-centered-cubic lattices. Finally, we explain how to use the KKR-NLCPA formalism to calculate observable quantities, such as the configurationally averaged density of states, for DFT calculations. In order to illustrate the improvements over the conventional KKR-CPA, in Sec. III we present results (configurationally averaged density of states) for the application of the formalism to a one-dimensional model. However, we emphasize that the formalism presented is fully tractable for realistic three-dimensional systems.

II. FORMALISM

A. The KKR-CPA

For the sake of clarity, we begin by briefly summarizing the idea of the conventional KKR-CPA[18,19] method. The path operator equation describing the scattering of an electron in a general array of nonoverlapping potentials, centered on site positions $\{\mathbf{R}_i\}$, is given by

$$\underline{\tau}^{ij}=\underline{t}^{i}\delta_{ij}+\sum_{k\neq i}\underline{t}^{i}\underline{G}(\mathbf{R}^{ik})\underline{\tau}^{kj}, \tag{1}$$

where the underscore denotes a matrix in angular momentum space with the usual angular momentum indices l,m; and $\mathbf{R}^{ij}=\mathbf{R}_i-\mathbf{R}_j$ is the position vector connecting sites i and j. For spherically symmetric scatterers, the individual t matrices are diagonal; i.e., $\underline{t}^{i}=t^{i}_{lm}\delta_{ij}\delta_{lm,l'm'}$, but the structure constants $G_{lm,l'm'}(\mathbf{R}^{ik})$ are not. We shall be interested in situations where the lattice sites labeled by i and j form a regular array, an infinite lattice, but the single-site t matrices vary from site to site in a random fashion. If we consider the solution of Eq. (1) for all possible disorder configurations and then take its average, we arrive at an averaged path operator $\overline{\underline{\tau}}^{ij}$ that is translationally invariant. In practice, it is not computationally feasible to average over every possible disorder configuration, nor is an equation that determines the averaged path operator $\overline{\underline{\tau}}^{ij}$ readily available in the form of Eq. (1). Under these circumstances, a way forward is to follow the strategy of ‘‘effective medium theories.’’[17,20] In the present context, a useful effective medium is that provided by an ordered array of effective scatterers described by the same t matrix $\hat{\underline{t}}$. In the KKR-CPA,[18,19] the scattering amplitude describing these effective scatterers is determined using the self-consistency condition that excess scattering off a single-site impurity embedded in such a medium should be zero on the average. As mentioned in the Introduction, while very successful in many applications, being a single-site approximation the CPA fails to take into account the effect of nonlocal potential correlations due to the disorder in the environment of each site.

B. Inclusion of nonlocal potential correlations

The first step in going beyond the KKR-CPA is to define what we will call the NLCPA effective medium by the following equation:

$$\hat{\underline{\tau}}^{ij}=\hat{\underline{t}}\,\delta_{ij}+\sum_{k\neq i}\hat{\underline{t}}\,\hat{\underline{G}}(\mathbf{R}^{ik})\hat{\underline{\tau}}^{kj}, \tag{2}$$

where a circumflex symbol denotes an NLCPA effective-medium quantity. Here we have defined NLCPA effective local t matrices $\hat{\underline{t}}$ and a new *effective propagator* by

$$\hat{\underline{G}}(\mathbf{R}^{ij})=\underline{G}(\mathbf{R}^{ij})+\hat{\underline{\alpha}}^{ij}. \tag{3}$$

This is composed of the usual free-space KKR structure constants $\underline{G}(\mathbf{R}^{ij})$ that account for the lattice structure plus a *translationally invariant* effective disorder term $\hat{\underline{\alpha}}^{ij}$ $(\equiv\hat{\alpha}^{ij}_{lm,l'm'})$. The matrix $\hat{\underline{\alpha}}^{ij}$ takes into account, in an averaged manner, the nonlocal correlations due to the disorder configurations.

Clearly, a cluster generalization of the KKR-CPA would involve determining the above NLCPA effective medium by requiring excess scattering off an impurity *cluster* of real potentials embedded in the effective medium to be zero on the average; and indeed this is the strategy adopted in the following section. However, the fact that $\hat{\underline{\alpha}}^{ij}$ is a translationally invariant effective-medium quantity means that it is diagonal in $\mathbf{k}$, the reciprocal space. In the present problem it is important to treat the theory in both real lattice and reciprocal lattice space consistently, and crucially we shall deal with this by a coarse-graining procedure.

C. Cluster generalization of the KKR-CPA

The first step is to consider a cluster of sites in the NLCPA effective medium. Denoting the sites within the cluster by capital letters, it can be shown (see Appendix A) that Eq. (2) can be rewritten as a cluster equation,

$$\hat{\underline{\tau}}^{IJ}=\hat{\underline{t}}^{IJ}_{cl}+\sum_{K,L}\hat{\underline{t}}^{IK}_{cl}\hat{\underline{\Delta}}^{KL}\hat{\underline{\tau}}^{LJ}, \tag{4}$$

with the effective *cluster t matrix* defined as

$$\underline{\hat{t}}^{IJ}_{cl}=\underline{\hat{t}}\,\delta_{IJ}+\sum_{K\neq I}\underline{\hat{t}}\,\underline{\widehat{G}}(\mathbf{R}^{IK})\underline{\hat{t}}^{KJ}_{cl}\,. \tag{5}$$

Equation (4) is simply a rearrangement of Eq. (2), so that the site matrix elements of all matrices involve the cluster sites only. The cluster t matrix $\underline{\hat{t}}^{IJ}_{cl}$ describes the scattering within a cluster and $\underline{\hat{\tau}}^{IJ}$ takes account of all scatterings outside the cluster via the effective *cluster renormalized interactor*[5,20] $\underline{\hat{\Delta}}^{IJ}$. Nevertheless, since $\underline{\widehat{G}}(\mathbf{R}^{IJ})=\underline{G}(\mathbf{R}^{IJ})+\underline{\hat{\alpha}}^{IJ}$, it is clear that the cluster t matrix also includes nonlocal correlations between the cluster sites.

It should be stressed that $\underline{\hat{\Delta}}^{IJ}$ describes those paths from the cluster site I to the cluster site J, which only involve intermediate sites outside the cluster. It is independent of the contents of the cluster and can be viewed as describing the effective medium from which the cluster has been removed, i.e., replaced by a *cavity*. We may now define an ‘‘impurity cluster’’ embedded in the effective medium simply by filling up this cavity with a particular configuration of site potentials. Clearly, the path operator for sites I,J belonging to such an impurity cluster is given by

$$\underline{\tau}^{IJ}_{imp}=\underline{t}^{IJ}_{cl,imp}+\sum_{K,L}\underline{t}^{IK}_{cl,imp}\underline{\hat{\Delta}}^{KL}\underline{\tau}^{LJ}_{imp}\,, \tag{6}$$

with the impurity cluster t matrix defined by

$$\underline{t}^{IJ}_{cl,imp}=\underline{t}^{I}\delta_{IJ}+\sum_{K\neq I}\underline{t}^{I}\underline{G}(\mathbf{R}^{IK})\underline{t}^{KJ}_{cl,imp}\,. \tag{7}$$

For a cluster containing N_c sites, each scattering according to $\underline{t}^{A}$ or $\underline{t}^{B}$, there are 2^{N_c} possible impurity cluster configurations.

We are now in a position to generalize the usual CPA self-consistency condition to determine our approximation to the exact configurationally averaged medium described by $\bar{\underline{\tau}}^{IJ}$, namely, the NLCPA effective medium described by $\underline{\hat{\tau}}^{IJ}$. This follows by considering for each configuration the impurity cluster path operator for paths starting and ending on the impurity cluster sites and demanding that the average over all configurations be equal to the path operator for the NLCPA effective medium itself, i.e.,

$$\langle\underline{\tau}^{IJ}_{imp}\rangle=\underline{\hat{\tau}}^{IJ}. \tag{8}$$

The important point to note is that unlike many other self-consistent cluster theories such as the molecular coherent-potential approximation[21,22] (MCPA) and extensions, here $\underline{\hat{\tau}}^{IJ}$ and $\underline{\hat{t}}$ correspond to an effective medium that is invariant under translation from site to site and hence does not yield spurious gaps in the band structure, which could affect the calculation of transport properties, etc.[5] This is a consequence of our definition of the nonlocal correlation terms $\underline{\hat{\alpha}}^{ij}$ as translationally invariant. To preserve this periodicity, during each self-consistency cycle we must have

$$\underline{\hat{\tau}}^{IJ}=\frac{1}{\Omega_{BZ}}\int_{\Omega_{BZ}}d\mathbf{k}[\underline{\hat{t}}^{-1}-\underline{\hat{\alpha}}(\mathbf{k})-\underline{G}(\mathbf{k})]^{-1}e^{i\mathbf{k}(\mathbf{R}_I-\mathbf{R}_J)}. \tag{9}$$

This can be seen by applying the usual lattice Fourier transform to Eq. (2) and then considering the cluster sites I,J. Clearly, to carry out the above integration numerically, we must have a specific representation of the function $\underline{\hat{\alpha}}(\mathbf{k})$. Following the central idea of the DCA, we proceed by coarse graining $\underline{\hat{\alpha}}(\mathbf{k})$ over the Brillouin zone. Unlike many other attempts,[5] this approach has been shown to be fully causal.[7]

D. Implementation—coarse graining of the Brillouin zone

Due to the finite size N_c of the cluster in real space, the differences in distance between the cluster sites correspond to a set of N_c cluster momenta $\{\mathbf{K}_n\}$ in reciprocal space according to the relation

$$\frac{1}{N_c}\sum_{\mathbf{K}_n}e^{i\mathbf{K}_n(\mathbf{R}_I-\mathbf{R}_J)}=\delta_{IJ}\,. \tag{10}$$

These $\{\mathbf{K}_n\}$ are at the centers of a set of N_c reciprocal-space patches that coarse grain the first Brillouin zone of the lattice. Earlier it was noted that the effective cluster t matrix also includes nonlocal correlation terms $\underline{\hat{\alpha}}^{IJ}$ acting between the cluster sites. We use the above relation to coarse grain $\underline{\hat{\alpha}}(\mathbf{k})$ as follows:

$$\underline{\hat{\alpha}}^{IJ}=\frac{1}{N_c}\sum_{\mathbf{K}_n}\underline{\hat{\alpha}}(\mathbf{K}_n)e^{i\mathbf{K}_n(\mathbf{R}_I-\mathbf{R}_J)}, \tag{11}$$

$$\underline{\hat{\alpha}}(\mathbf{K}_n)=\sum_{J\neq I}\underline{\hat{\alpha}}^{IJ}e^{-i\mathbf{K}_n(\mathbf{R}_I-\mathbf{R}_J)}. \tag{12}$$

Since the NLCPA maps the effective lattice problem to that of a self-consistently embedded impurity cluster problem, the fundamental assumption we make is that provided we are aiming to reproduce these correlations of finite range in the effective lattice, we may take the above coarse-grained values $\underline{\hat{\alpha}}(\mathbf{K}_n)$ to be a good approximation to $\underline{\hat{\alpha}}(\mathbf{k})$ for the effective lattice. In short, $\underline{\hat{\alpha}}(\mathbf{k})=\underline{\hat{\alpha}}(\mathbf{K}_n)$ if $\mathbf{k}$ is in the nth reciprocal-space patch. This is discussed more formally in Appendix B.

The next step is to define the ‘‘coarse-grain averaged’’ reciprocal-space matrix elements for the effective-medium path operator by

$$\underline{\hat{\tau}}(\mathbf{K}_n)=\frac{N_c}{\Omega_{BZ}}\int_{\Omega_{\mathbf{K}_n}}d\mathbf{k}[\underline{\hat{t}}^{-1}-\underline{\hat{\alpha}}(\mathbf{K}_n)-\underline{G}(\mathbf{k})]^{-1}, \tag{13}$$

where each integral is over the reciprocal-space patch $\Omega_{\mathbf{K}_n}$ of volume N_c/Ω_{BZ} surrounding the point $\mathbf{K}_n$. This is straightforward since each $\underline{\hat{\alpha}}(\mathbf{K}_n)$ is constant within its coarse-graining patch. Defining transformations relating the real-space and coarse-grained reciprocal-space matrix elements by

$$\hat{\underline{\tau}}^{IJ}=\frac{1}{N_c}\sum_{\mathbf{K}_n}\hat{\underline{\tau}}(\mathbf{K}_n)e^{i\mathbf{K}_n(\mathbf{R}_I-\mathbf{R}_J)}, \tag{14}$$

$$\hat{\underline{\tau}}(\mathbf{K}_n)=\sum_J \hat{\underline{\tau}}^{IJ}e^{-i\mathbf{K}_n(\mathbf{R}_I-\mathbf{R}_J)} \tag{15}$$

means that the real-space effective-medium path operator for sites I,J within the cluster is now given by

$$\hat{\underline{\tau}}^{IJ}=\frac{1}{\Omega_{BZ}}\sum_{\mathbf{K}_n}\left(\int_{\Omega_{\mathbf{K}_n}}d\mathbf{k}[\hat{\underline{t}}^{-1}-\hat{\underline{\alpha}}(\mathbf{K}_n)-\underline{G}(\mathbf{k})]^{-1}e^{i\mathbf{K}_n(\mathbf{R}_I-\mathbf{R}_J)}\right), \tag{16}$$

which we use to replace Eq. (9), and we can now iterate to self-consistency until Eqs. (8) and (16) are satisfied.

Finally, note that the NLCPA reduces to the CPA for $N_c=1$. In this limit, the nonlocal correlation terms $\hat{\underline{\alpha}}^{IJ}$ vanish and the NLCPA effective t matrix becomes equal to the usual CPA effective t matrix. The NLCPA becomes exact as $N_c\rightarrow\infty$, where $\mathbf{K}_n\rightarrow\mathbf{k}$ and nonlocal correlations over all length scales are treated. For clarity, the full KKR-NLCPA algorithm is now summarized below.

E. KKR-NLCPA algorithm

All real-space matrices in the algorithm are supermatrices (denoted by double underscores) in cluster site and angular momentum space. For a particular energy E, we have the following.

(1) Make a guess for the effective cluster t matrix $\hat{\underline{t}}_{cl}^{IJ}$ for the first iteration. Do this by placing an average t matrix, $\overline{\underline{t}}=P(A)\underline{t}^A+P(B)\underline{t}^B$ [where $P(A)$ is the probability of a site being occupied by an A atom), on each cluster site; and for the site-to-site propagation terms in the cluster, use the free-space structure constants, i.e., set $\hat{\underline{\alpha}}^{IJ}=0$.

(2) Calculate $\hat{\underline{\alpha}}^{IJ}$ using Eq. (5), i.e.,

$$\hat{\underline{\underline{\alpha}}}=\hat{\underline{\underline{t}}}^{-1}-\hat{\underline{\underline{t}}}_{cl}^{-1}-\underline{\underline{G}},$$

where $\hat{\underline{\underline{t}}}^{-1}$ is the diagonal part of $\hat{\underline{\underline{t}}}_{cl}^{-1}$. For the first iteration, $\hat{\underline{\alpha}}^{IJ}$ will of course be zero.

(3) Convert the matrix elements $\hat{\underline{\alpha}}^{IJ}$ to coarse-grained reciprocal space using Eq. (12).

(4) Calculate the coarse-grained matrix elements $\hat{\underline{\tau}}(\mathbf{K}_n)$ using Eq. (13) and convert them to real space using Eq. (14).

(5) Calculate $\hat{\underline{\Delta}}^{IJ}$ by solving Eq. (4), i.e.,

$$\underline{\underline{\Delta}}=\underline{\underline{t}}_{cl}^{-1}-\underline{\underline{\tau}}^{-1}.$$

(6) Calculate $\underline{\tau}_{imp}^{IJ}$ for each impurity cluster configuration using Eq. (6) and average over all 2^{N_c} configurations to obtain a new effective path operator at the cluster sites $\hat{\underline{\tau}}^{IJ}$.

(7) Calculate the new cluster t matrix $\hat{\underline{t}}_{cl}^{IJ}$ by solving Eq. (4) using $\hat{\underline{\tau}}^{IJ}$ above and $\hat{\underline{\Delta}}^{IJ}$ from step 5, i.e.,

$$\underline{\underline{t}}_{cl}=(\underline{\underline{\tau}}^{-1}+\underline{\underline{\Delta}})^{-1}.$$

(8) Compare the new cluster t-matrix elements $\hat{\underline{t}}_{cl}^{IJ}$ with those in step 1. If they are not equal to within the desired accuracy, repeat as necessary steps $2\rightarrow 8$ using the new cluster t matrix until convergence within the desired accuracy is achieved.

Note that the integrations over the reciprocal space patches in step 4 only involve the inversion of a matrix in angular momentum space, and therefore the computational time is not significantly increased over the conventional KKR-CPA regardless of cluster size. This is in contrast to many other attempts such as the MCPA, where the integration over the Brillouin zone requires the inversion of a supermatrix in cluster site and angular momentum space for each value of $\mathbf{k}$. We also draw attention to the recent work of Maier and Jarrell[22] where the DCA algorithm has been shown to converge more quickly than the MCPA algorithm, with corrections of order $1/L^2$ (where L is the linear size of the cluster).

F. The cluster momenta $\{\mathbf{K}_n\}$

Since the NLCPA maps the impurity cluster problem to the effective lattice problem in reciprocal space, it is important to realize that the real-space cluster must have periodic boundary conditions, i.e., must preserve the translational symmetry of the lattice. Moreover, as explained in Ref. 9, in order to obtain suitable reciprocal-space patches centered at the cluster momenta $\{\mathbf{K}_n\}$, we must select the real-space cluster sites by surrounding them with a "tile" of size L^D (where D is the dimension) which preserves the full point-group symmetry of the lattice, and only clusters that satisfy this requirement are allowed.

The method for finding the corresponding cluster momenta $\{\mathbf{K}_n\}$ satisfying Eq. (10) for a simple two-dimensional square lattice has been described in Ref. 9. Here we generalize this method to the case of three-dimensional simple cubic (sc), body-centered-cubic (bcc), and face-centered-cubic (fcc) lattices commonly found in real disordered alloys. For the trivial case of $N_c=1$, the real-space tiles with the required symmetry would simply be Wigner-Seitz cells surrounding each lattice point. For larger cluster sizes, we may take the tiles to be simple cubes of volume L^3 for each of these lattices. The smallest possible cluster sizes are given by considering $L=a$ (where a is the lattice constant), and this yields $N_c=1$ for sc (trivial), $N_c=2$ for bcc, and $N_c=4$ for fcc lattices. The next set of allowed cluster sizes is given by considering $L=2a$; and this yields $N_c=8$, $N_c=16$, and $N_c=32$ for sc, bcc, and fcc lattices, respectively.

The next step is to consider the "principal tiling vectors" $\{\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3\}$, where $l\mathbf{a}_1+m\mathbf{a}_2+n\mathbf{a}_3$ for integers l,m,n map out the centers of the real-space tiles. Applying the usual reciprocal-space transformations of the form $\mathbf{b}_1=2\pi(\mathbf{a}_2\times\mathbf{a}_3)/[\mathbf{a}_1\cdot(\mathbf{a}_2\times\mathbf{a}_3)]$, etc. gives us principal "coarse-grained" reciprocal-space vectors $\{\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3\}$. We take N_c

TABLE I. Examples of sets of $\mathbf{R}_I$ and $\mathbf{K}_n$ values for lattices of the sc, bcc, and fcc type.

Lattice	N_c	Cube edge L	$\mathbf{R}_I$ values (units of lattice constant a)	$\mathbf{K}_n$ values (units of π/a)
sc	1	a	(0,0,0)	(0,0,0)
	8	$2a$	$\{\mathbf{R}_I^{sc}\}=\{(0,0,0),\ (0,0,1),$ $(0,1,0),\ (0,1,1),\ (1,0,0),$ $(1,0,1),\ (1,1,0),\ (1,1,1)\}$	$\{\mathbf{K}_n^{sc}\}=\{(0,0,0),\ (0,0,1),$ $(0,1,0),\ (0,1,1),\ (1,0,0),$ $(1,0,1),\ (1,1,0),\ (1,1,1)\}$
bcc	2	a	$(0,0,0),\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(0,0,0), (2,0,0)
	16	$2a$	$\{\mathbf{R}_I^{sc}\},\ \{\mathbf{R}_I^{sc}+(\frac{1}{2},\frac{1}{2},\frac{1}{2})\}$	$\{\mathbf{K}_n^{sc}\},\ \{\mathbf{K}_n^{sc}+(2,0,0)\}$
fcc	4	a	$(0,0,0),\ (\frac{1}{2},0,\frac{1}{2}),\ (\frac{1}{2},\frac{1}{2},0),\ (0,\frac{1}{2},\frac{1}{2})$	(0,0,0), (2,0,0), (0,2,0), (0,0,2)
	32	$2a$	$\{\mathbf{R}_I^{sc}\},\ \{\mathbf{R}_I^{sc}+(\frac{1}{2},0,\frac{1}{2})\},$ $\{\mathbf{R}_I^{sc}+(\frac{1}{2},\frac{1}{2},0)\},\ \{\mathbf{R}_I^{sc}+(0,\frac{1}{2},\frac{1}{2})\}$	$\{\mathbf{K}_n^{sc}\},\ \{\mathbf{K}_n^{sc}+(2,0,0)\}$ $\{\mathbf{K}_n^{sc}+(0,2,0)\},\ \{\mathbf{K}_n^{sc}+(0,0,2)\}$

nonequivalent vectors (i.e., which do not differ by a reciprocal-lattice vector) of the form $l\mathbf{b}_1+m\mathbf{b}_2+n\mathbf{b}_3$ for integers l,m,n to be our set of cluster momenta $\{\mathbf{K}_n\}$, and these will satisfy Eq. (10). The reciprocal-space patches surrounding these cluster momenta will be simple cubes of equal volume $(2\pi/L)^3$, which together will fill out a volume of the size of the first Brillouin zone; i.e., $(2\pi/a)^3$ for sc, $2(2\pi/a)^3$ for bcc, and $4(2\pi/a)^3$ for fcc lattices, respectively. Integrating over these patches is equivalent to integrating over the first Brillouin zone of the lattice since $\mathbf{K}_n$ values and parts of patches lying outside of the first Brillouin zone can be translated through reciprocal lattice vectors (of the sc, bcc, or fcc lattice as appropriate) to lie within the first Brillouin zone. In Table I we give some examples of sets of $\mathbf{R}_I$ and corresponding $\mathbf{K}_n$ values obtained using the above method.

G. Short-range order

The principal advantage of the KKR-NLCPA over the conventional KKR-CPA is that it can be implemented for alloys in which short-range ordering or clustering is present. To deal with this situation, one must include an appropriate weighting for each of the 2^{N_c} impurity cluster configurations in step 6 of the algorithm. Note that such short-range order will not destroy the translational invariance because it will be restored by the configurational averaging. However, when using some method to weight the configurations, it is important to bear in mind the periodic boundary conditions imposed on the cluster as explained in the preceding section. To illustrate the above feature of the theory, we will describe short-range order with a one-dimensional example later in this paper.

H. Calculating observables

In order to calculate observables such as the configurationally averaged densities and density of states, we need to know the configurationally averaged Green's function calculated within the NLCPA. The expression for the Green's function before averaging is given by

$$G(E,\mathbf{r}_i,\mathbf{r}_j')=\sum_{LL'} Z_L^i(E,\mathbf{r}_i)\tau_{LL'}^{ij}Z_{L'}^j(E,\mathbf{r}_j') - \sum_L Z_L^i(E,\mathbf{r}_i)J_L^i(E,\mathbf{r}_i')\delta_{ij}, \tag{17}$$

where $L(=l,m)$ is an angular momentum index and $\mathbf{r}_i(\mathbf{r}_j')$ lies within the unit cell centered at site $i(j)$. $Z_L^i(E,\mathbf{r}_i)$ and $J_L^i(E,\mathbf{r}_i)$ are the regular and irregular solutions,[23] respectively, of the single-site problem at site i. In the following section we show calculations for the configurationally averaged density of states for a one-dimensional model, and so here we demonstrate explicitly how to take the configurational average of the site-diagonal Green's function. It should be stressed that unlike in calculations based on tight-binding models, in the present multiple-scattering theory we solve for and describe the site-to-site fluctuations of the "orbitals" $Z_L^i(E,\mathbf{r}_i)$. In short, we can calculate the density $\mathbf{r}$ point by $\mathbf{r}$ point. It is this feature of the present theory which requires the following careful averaging procedure.

The first step is to consider $\mathbf{r}$ and $\mathbf{r}'$ in the neighborhood of a cluster site I. Denoting a configuration of the remaining cluster sites by γ, as a generalization of Ref. 23 we first average over the subset of possible lattice structures that leave the potential in site I fixed:

$$\begin{aligned}\langle G(E,\mathbf{r},\mathbf{r}')\rangle_I &=\sum_{LL'} Z_L^I(E,\mathbf{r}_I)\left(\sum_{\gamma} P(\gamma|I)\langle\tau_{LL'}^{II}\rangle_{I,\gamma}\right)\\ &\quad\times Z_{L'}^I(E,\mathbf{r}_I')-\sum_L Z_L^I(E,\mathbf{r}_I)J_L^I(E,\mathbf{r}_I').\end{aligned} \tag{18}$$

Here $\langle\tau_{LL'}^{II}\rangle_{I,\gamma}$ is the path operator for paths starting and ending at site I conditionally averaged so that the potential on site I is known (to either be of type A or B), and the configuration of the remaining sites in the cluster is known to be γ. $P(\gamma|I)$ is the probability that the configuration γ of the remaining cluster sites occurs, given the type of potential at site I. The final step is to average over the possible occupants of site I itself:

$$\begin{aligned}\langle G(E,\mathbf{r},\mathbf{r}')\rangle = \sum_{LL'} \Bigg[& P(A) Z_L^A(E,\mathbf{r}_I) \Bigg(\sum_{\gamma} P(\gamma|A) \\ & \times \langle \tau_{LL'}^{II} \rangle_{A,\gamma} \Bigg) Z_{L'}^A(E,\mathbf{r}_I') + P(B) Z_L^B(E,\mathbf{r}_I) \\ & \times \Bigg(\sum_{\gamma} P(\gamma|B) \langle \tau_{LL'}^{II} \rangle_{B,\gamma} \Bigg) Z_{L'}^B(E,\mathbf{r}_I') \Bigg] \\ & - \sum_L [P(A) Z_L^A(E,\mathbf{r}_I) J_L^A(E,\mathbf{r}_I') \\ & + P(B) Z_L^B(E,\mathbf{r}_I) J_L^B(E,\mathbf{r}_I')]. \end{aligned} \tag{19}$$

Here $P(A)$ and $P(B)$ are the probablities that site I is an A atom and a B atom, respectively (i.e., the concentrations of A and B atoms in the material). This can be rewritten as

$$\begin{aligned}\langle G(E,\mathbf{r},\mathbf{r}')\rangle & \\ = \sum_{LL'} \Bigg[& \sum_{\gamma} P(A,\gamma) Z_L^A(E,\mathbf{r}_I) \langle \tau_{LL'}^{II} \rangle_{A,\gamma} Z_{L'}^A(E,\mathbf{r}_I') \\ & + \sum_{\gamma} P(B,\gamma) Z_L^B(E,\mathbf{r}_I) \langle \tau_{LL'}^{II} \rangle_{B,\gamma} Z_{L'}^B(E,\mathbf{r}_I') \Bigg] \\ & - \sum_L [P(A) Z_L^A(E,\mathbf{r}_I) J_L^A(E,\mathbf{r}_I') \\ & + P(B) Z_L^B(E,\mathbf{r}_I) J_L^B(E,\mathbf{r}_I')], \end{aligned} \tag{20}$$

where (A,γ) and (B,γ) denote cluster configurations with an A atom and B atom on site I, respectively. The above expression is still exact at this stage, however it can be simplified using the NLCPA. In this approximation, $\langle \tau_{LL'}^{II} \rangle_{I,\gamma}$ is constructed using an "impurity" cluster of configuration (I,γ) embedded in the NLCPA effective medium. By using Eq. (4) to eliminate the cluster renormalized interactor from Eq. (6), this is given by

$$\langle \tau_{LL'}^{II} \rangle_{I,\gamma} = [(\hat{\underline{\underline{\tau}}}^{-1} + \underline{\underline{t}}_{cl,imp}^{-1} - \hat{\underline{\underline{t}}}_{cl}^{-1})^{-1}]_{LL'}^{II}, \tag{21}$$

where the impurity cluster t matrix $\underline{\underline{t}}_{cl,imp}$ has configuration (I,γ), and the notation implies taking the I,Ith site and L,L'th angular momentum element of the supermatrix on the right-hand side.

It does not matter which cluster site is chosen to be site I in all the above formulas as $\hat{G}(E,\mathbf{r},\mathbf{r}')$, the resulting approximation to $\langle G(E,\mathbf{r},\mathbf{r}')\rangle$, is a translationally invariant quantity. The density of states per site is given by

$$\rho(E) = \frac{-1}{\pi} \mathrm{Im} \int_{\Omega_I} \hat{G}(E,\mathbf{r},\mathbf{r}) d\mathbf{r}, \tag{22}$$

where the integral is over Ω_I, the volume of site I.

III. RESULTS FOR ONE-DIMENSIONAL MODEL

The multiple-scattering theory in three dimensions envisions three-dimensional potential wells of finite range surrounding the atomic nuclei, the famous muffin-tin potential. A very useful caricature of this realistic situation can be constructed in one dimension. Evidently, in this case the unit cell is a line segment and the potential wells are described by a function $V(x)$ of one spatial variable only. Interestingly, one may regard the sign of x as an angle and develop an analog of the three-dimensional angular momentum expansion of the usual KKR theory. Since it was first formulated by Butler,[24] it has been made good use of by a number of authors, for example, see Refs. 25–27. While it is computationally simple, as one might expect, it is formally identical to KKR in three dimensions. For example, there are two "angular momentum" values $L=0,1$ (and hence all NLCPA supermatrices in the algorithm have dimension $2N_c$), and there is an explicit expression for the structure constants. For a detailed description, see Refs. 24 and 25.

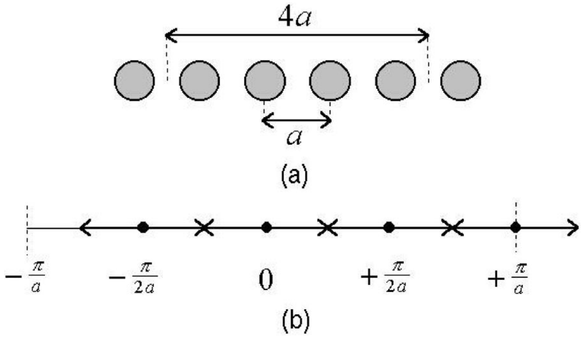

FIG. 1. A one-dimensional tile for a one-dimensional effective four-site ($N_c=4$) cluster is shown in (a). Its length L is $4a$, where a is the lattice constant. The corresponding set of cluster momenta (denoted by dots) and reciprocal-space patches of length $2\pi/L$ in relation to the first Brillouin zone are shown in (b).

For a cluster of size N_c, the one-dimensional reciprocal-space patches are simply defined by the points

$$\mathbf{K}_n = \frac{(2n-N_c)\pi}{N_c a},$$

where a is the lattice constant and $n=1,\ldots,N_c$. As an example, the real-space "one-dimensional tiles" and reciprocal-space patches for a four-site ($N_c=4$) cluster are shown in Fig. 1.

We have carried out extensive numerical calculations of the configurationally averaged density of states for a one-dimensional alloy over a wide range of parameters. In all cases we have found that the KKR-NLCPA systematically improves the density of states with increasing cluster size compared to the conventional KKR-CPA.

As a simple illustration we set the lattice constant to be $a=6.00$ a.u. and potential-well radius to be $r_{MT}=2.25$ a.u. for each of the constituent potentials for A and B sites, which are square potential wells of depths -1.2 Ry and -0.6 Ry, respectively. The concentration of A sites is taken to be 80%. The density of states for the electrons in lattices of purely A sites and purely B sites together with the CPA result for the $A_{80}B_{20}$ alloy is shown in Fig. 2. In Fig. 3 we show for comparison the results for a four-site supercell calculation. This is obtained by considering an infinite periodic supercell containing four sites of a particular configuration and then aver-

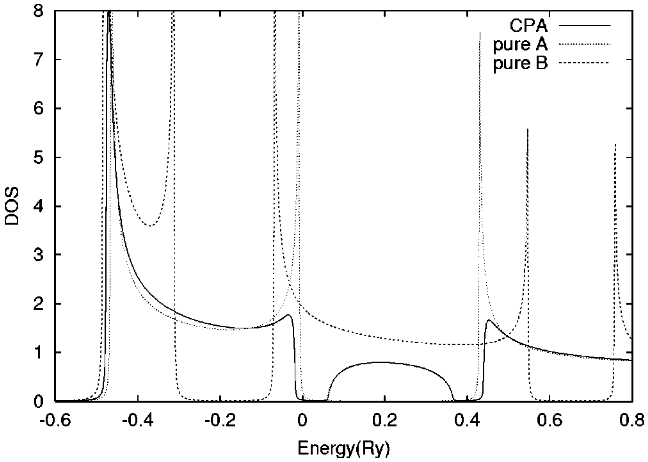

FIG. 2. Density of states for a one-dimensional model. Results shown are for a pure A lattice, a pure B lattice, and a KKR-CPA calculation for an $A_{80}B_{20}$ alloy.

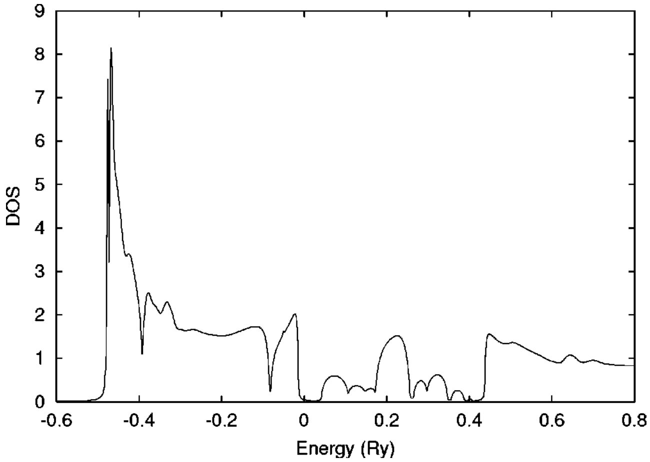

FIG. 4. A four-site ($N_c=4$) KKR-NLCPA calculation for the $A_{80}B_{20}$ alloy. Notice the improved structure and the partial filling in of the band gaps compared with the KKR-CPA calculation in Fig. 2.

aging over all 2^4 possible configurations. The supercell, calculation is not the exact result due to the finite size of the supercell but it gives an indication of the type of structure to expect if we are to improve upon the CPA. A KKR-NLCPA calculation with a cluster size of 4 ($N_c=4$) is shown in Fig. 4. It is evident that much of the structure missing from the CPA calculation, which can be associated with energy bands of particular configurations of the supercell, is reproduced here. States also appear in the band gaps at either side of the impurity band centered at 0.2 Ry, which are absent in the CPA calculation. This is because the states near the band edges are the contributions of large clusters of like atoms, and these cannot be dealt with by a single-site theory such as the CPA. To investigate this further, an eight-site ($N_c=8$) calculation is shown in Fig. 5. Clearly, with increasing cluster size, more and more states enter the band gaps.

Next we illustrate the ability of the KKR-NLCPA to take into account the effects of short-range order. As mentioned earlier, the KKR-NLCPA can be implemented for arbitrary ensembles including those in which the occupancy of a site by an A or B atom is correlated to that of neighboring sites. As a simple example, we increase the probablity of an atom occupying a site by a factor β if it follows a like atom, and decrease its probability by the same factor if it follows an unlike atom in the one-dimensional cluster. Thus positive values of β correspond to short-range clustering and negative values of β correspond to short-range ordering. As an example, for a four-site impurity cluster of configuration $ABBA$, we have $P(ABBA)=[P(A)+\beta][P(B)-\beta][P(B)+\beta][P(A)-\beta]$ where we have made use of the periodic boundary conditions imposed on the cluster. In Fig. 6 we show a four-site ($N_c=4$) KKR-NLCPA calculation for the density of states using the same parameters as before, along with short-range order parameter values $\beta=-0.1$, $\beta=0.0$, and $\beta=+0.1$. Peaks which increase or decrease can be identified with specific cluster configurations, and the increases or decreases in the amplitude of the peaks are consistent with the increased or decreased cluster probabilities.

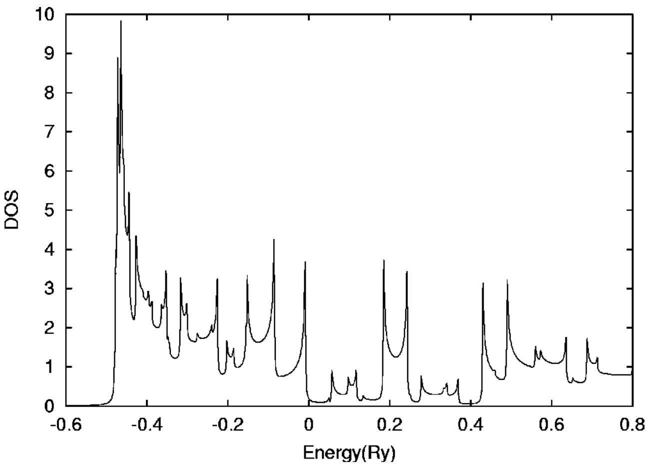

FIG. 3. A four-site ($N_c=4$) supercell calculation for the $A_{80}B_{20}$ alloy obtained by averaging over all 2^4 possible configurations of an infinite periodic supercell containing four sites.

IV. CONCLUSIONS

We have presented the formalism for the KKR-NLCPA method which systematically improves upon the conventional KKR-CPA for describing disordered systems on the basis of a first-principles description of the crystal potential. We have demonstrated its use on a one-dimensional model and illustrated in detail the necessary coarse-graining procedure for real three-dimensional lattices. We have also shown how to calculate observable quantities with a view to combining the KKR-NLCPA with density-functional theory. In the explicit calculations, the emphasis was on the improved structure in the density of states with increasing cluster size due to nonlocal correlations, and on a simple example of the ability of the KKR-NLPCA to model the effects of compositional short-range order.

In order for disordered systems to receive a “first-principles” description, electronic density-functional theory[16] (DFT) needs to be combined with treatments of dis-

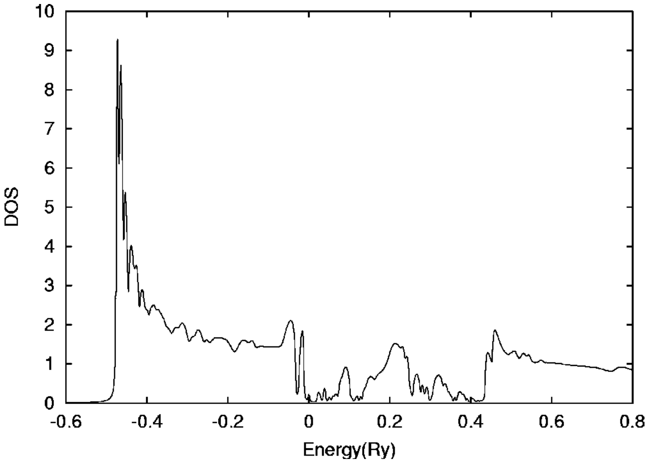

FIG. 5. An eight-site ($N_c=8$) KKR-NLCPA calculation for the $A_{80}B_{20}$ alloy. Notice the increasing density of states inside the CPA band gaps.

order. The self-consistent-field Korringa-Kohn-Rostocker coherent-potential approximation (SCF-KKR-CPA)[28,29] approach is a "first-pass" way at doing this, and has been applied to a wide range of disordered alloys.[30,31] It has also been adapted for the problem of itinerant magnets at finite temperatures whose "disordered local-moment" spin fluctuations are handled using the CPA.[32,33] In principle, a DFT calculation of a disordered system should mean that separate SCF calculations are carried out to minimize the total energy for each disorder configuration individually, and then an average taken over all disorder configurations. This is, of course, intractable, and the strategy behind SCF-KKR-CPA calculations has been to minimize a functional for the averaged energy in terms of partially averaged charge (and spin) densities, i.e., the average of charge densities arising from all configurations that have either an A or a B atom on one site. From this approach, however, it is not straightforward to include local environment effects such as electrostatic, "charge-correlation"[31,34,35] Madelung, and local lattice displacement effects in alloys or indeed short-range order effects in general. For disordered alloys, the implementation requires the solution of the Kohn-Sham equations for electrons moving in the disordered arrays of the effective potentials associated with A and B sites which are insensitive to their environments. In the context of finite temperature magnetism, it means that the thermally induced spin fluctuations must be characterized as "local moments" associated with single sites and not larger clusters. In this paper we show how these serious omissions may be rectified by presenting a scheme within the KKR framework, which goes systematically beyond the CPA.

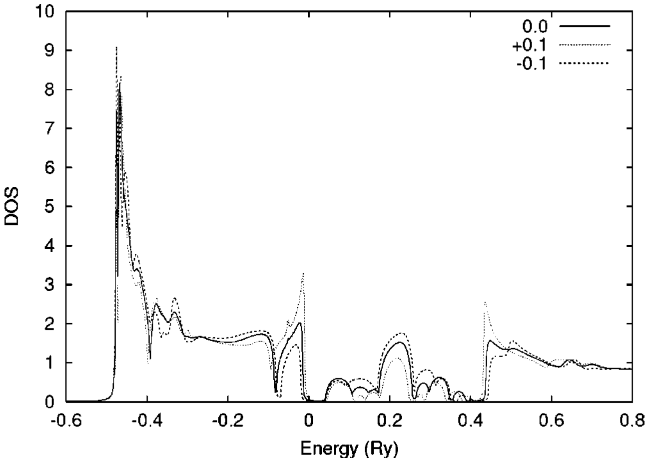

FIG. 6. Effects of short-range ordering ($\beta=-0.1$) and clustering ($\beta=+0.1$) on the four-site ($N_c=4$) KKR-NLCPA calculation for the $A_{80}B_{20}$ alloy.

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APPENDIX A:

Consider a finite-sized cluster C of sites in the effective medium. Equation (2) for sites i,j belonging to the cluster can be written in the form

$$\underline{\hat{\tau}}^{ij}=\underline{\hat{t}}\delta_{ij}+\sum_{k\in C}\underline{\hat{t}}\,\underline{\hat{G}}(\mathbf{R}^{ik})\underline{\hat{\tau}}^{kj}+\sum_{k\notin C}\underline{\hat{t}}\,\underline{\hat{G}}(\mathbf{R}^{ik})\underline{\hat{\tau}}^{kj}, \qquad \text{(A1)}$$

where the sum over all sites k has been split into those involving sites k within the cluster and sites k outside of the cluster. It can be shown[5,36] that

$$\sum_{k\notin C}\underline{\hat{G}}(\mathbf{R}^{ik})\underline{\hat{\tau}}^{kj}=\sum_{l\in C}\underline{\hat{\Delta}}^{il}\underline{\hat{\tau}}^{lj}, \qquad \text{(A2)}$$

with the effective cluster renormalized interactor $\underline{\hat{\Delta}}^{ij}$ given by the locator expansion

$$\underline{\hat{\Delta}}^{ij}=\sum_{k\notin C}\underline{\hat{G}}(\mathbf{R}^{ik})\underline{\hat{t}}\,\underline{\hat{G}}(\mathbf{R}^{kj})$$

$$+\sum_{k\notin C,l\notin C}\underline{\hat{G}}(\mathbf{R}^{ik})\underline{\hat{t}}\,\underline{\hat{G}}(\mathbf{R}^{kl})\underline{\hat{t}}\,\underline{\hat{G}}(\mathbf{R}^{lj})+\cdots. \qquad \text{(A3)}$$

Inserting Eq. (A2) into Eq. (A1) and using the notation that cluster sites are denoted by capital letters gives

$$\underline{\hat{\tau}}^{IJ}=\underline{\hat{t}}\delta_{IJ}+\sum_{K}\underline{\hat{t}}(\underline{\hat{G}}(\mathbf{R}^{IK})+\underline{\hat{\Delta}}^{IK})\underline{\hat{\tau}}^{KJ}, \qquad \text{(A4)}$$

which can be rearranged as

$$\underline{\hat{\tau}}^{IJ}=\underline{\hat{t}}_{cl}^{IJ}+\sum_{K,L}\underline{\hat{t}}_{cl}^{IK}\underline{\hat{\Delta}}^{KL}\underline{\hat{\tau}}^{LJ} \qquad \text{(A5)}$$

to include the effective cluster t matrix given by Eq. (5).

APPENDIX B:

First we note that the correlations between the cluster sites that we are aiming to reproduce in the effective lattice are of a finite range, say $\lesssim L/2$, where L is the linear size of the tile surrounding the cluster sites (see Sec. II F). The next step is to divide or "coarse-grain" the first Brillouin zone of the lattice of N sites into $N_c = L^D$ patches of size $(2\pi/L)^D$ (where D is the dimension) centered at the cluster momenta $\{\mathbf{K}_n\}$. We now consider each coarse-grained value $\underline{\hat{\alpha}}(\mathbf{K}_n)$ to be the average of $\underline{\hat{\alpha}}(\mathbf{k})$ over the N/N_c lattice momenta $\tilde{\mathbf{k}}$ within the patch surrounding the point $\mathbf{K}_n$:

$$\underline{\hat{\alpha}}(\mathbf{K}_n) = \frac{N_c}{N} \sum_{\tilde{\mathbf{k}}} \underline{\hat{\alpha}}(\mathbf{K}_n + \tilde{\mathbf{k}}). \tag{B1}$$

The fundamental assumption we make is to take these coarse-grained values $\underline{\hat{\alpha}}(\mathbf{K}_n)$ to be a good approximation to $\underline{\hat{\alpha}}(\mathbf{k})$ for the effective lattice,[7] This is because according to Nyquist's sampling theorem[37] in order to reproduce correlations of a finite range $(L/2)$ in real space, we only need to sample the first Brillouin zone of the lattice at intervals of $2\pi/L$, i.e., at the cluster momenta $\{\mathbf{K}_n\}$. The real-space correlation terms $\underline{\hat{\alpha}}^{ij}(1-\delta_{ij})$ are cut off if the distance between i and j is outside the range of the cluster size. As $N_c \rightarrow \infty$, correlations over all length scales are treated since the maximum correlation length is proportional to the cluster size N_c.

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