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2006 J. Phys.: Condens. Matter 18 507

(http://iopscience.iop.org/0953-8984/18/2/012)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **18** (2006) 507–520 doi:10.1088/0953-8984/18/2/012

Effective medium super-cell approximation for interacting disordered systems: an alternative real-space derivation of generalized dynamical cluster approximation

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Received 13 July 2005, in final form 7 November 2005
Published 14 December 2005
Online at stacks.iop.org/JPhysCM/18/507

Abstract

We develop a generalized real-space effective medium super-cell approximation (EMSCA) method to treat the electronic states of interacting disordered systems. This method is general and allows randomness both in the on-site energies and in the hopping integrals. For a non-interacting disordered system, in the special case of randomness in the on-site energies, this method is equivalent to the non-local coherent potential approximation (NLCPA) derived previously. Also, for an interacting system the EMSCA method leads to the real-space derivation of the generalized dynamical cluster approximation (DCA) for a general lattice structure. We found that the original DCA and the NLCPA are two simple cases of this technique, so the EMSCA is equivalent to the generalized DCA where there is included interaction and randomness in the on-site energies and in the hopping integrals. All of the equations of this formalism are derived by using the effective medium theory in real space.

1. Introduction

Theoretical understanding of alloys and strongly correlated systems such as high temperature superconductors, heavy fermions and magnetism requires appropriate techniques to obtain their physical properties. Recently, using many body theory techniques, it has been shown that both alloys and strongly correlated systems in the infinite dimensional limit are mapped to a single site which is embedded in an effective medium [1–4]. This can be described by a restriction on the locality of self-energy, i.e., $\Sigma(i, j; \mathrm{i}\omega_n) = \Sigma(\mathrm{i}\omega_n)\delta_{ij}$. These single site techniques for strongly correlated systems and alloys systems are called the *dynamical mean field approximation* (DMFA) [5] and *coherent potential approximation* (CPA) [6, 7]

respectively. The single site nature of the infinite-dimensional limit implies that the inter-site correlations and inter-site multiple scattering are negligible. But in the ordinary dimensions, such as one, two and three, both inter-site correlation and inter-site multiple scattering have a significant contribution on the self-energy. Therefore not only is the self-energy not local but also it is very sensitive with respect to the dimension. In order to include such inter-site effects extensions of CPA were developed using the locator formalism [8–10]. In the propagator formalism the cluster CPA technique was developed by Nickel and Butler [11] where the self-energy is not causal. The molecular coherent potential approximation (MCPA) [12] is formulated in real space with open boundary conditions on a finite cluster which does not preserve the real lattice translational invariance [13]. Also for interacting systems the cellular dynamical mean field theory (CDMFT) [14] was developed in real space by dividing the real lattice into clusters. However, recently the dynamical cluster approximation (DCA) has been introduced for interacting systems [15]. A version of DCA has also been used to treat disordered systems [16]. This method improved the CPA by allowing weak wavevector dependence of the self-energy, $\Sigma(k;\omega)$. The DCA was originally derived on the basis of momentum conservation in the coarse grained first Brillouin zone (FBZ). Momentum conservation is applied only to the coarse grained wavevector $\mathbf{K}_n$ in the FBZ and in the corresponding Laue function. In this method a key computational step makes use of a Fourier like transformation of coarse grained wavevectors $\mathbf{K}_n$ to a real-space set of coordinates, $\mathbf{R}_n$. These coordinates were interpreted as the lattice sites of a real cluster of a real lattice. However, this connection was not established directly and their $\mathbf{K}_n$ are correct for a hyper cubic lattice structure.

Using effective medium theory in real space we have developed a non-local CPA (NLCPA) method [17]. In this method a cluster of impurities is embedded in an effective medium, such that all averaged clusters are equivalent and lattice periodicity is preserved. We also applied NLCPA as a real-space super-cell approximation to explain the resonance peak that appears in the density of states of substituted Zn impurity in the CuO_2 plane of $Bi_2Sr_2Ca_2Cu_3O_{8+\delta}$ [17]. A real-space super-cell approximation which is called the *effective medium super-cell approximation* (EMSCA) has been developed by us. We have applied this technique to a carbon nanotube alloy system. It has been found that the semiconducting gap of a zigzag single walled carbon nanotube, E_g, could be controlled by doping boron and nitrogen [18]. Here the EMSCA is extended to treat both disorder and interaction simultaneously. This method preserves both causality and translational invariance; it could be equivalent to the generalized DCA to include random hopping integrals. The EMSCA method leads to derivation of the DMFT and CPA for the case of ($N_c = 1$) and it is exact when number of lattice sites in the super-cell goes to infinity ($N_c \to \infty$). We show that neglecting the interaction between electrons in different super-cells, disorder multiple scattering by sites in different super-cells and also deviations of the hopping integrals, $\delta t_{ij}^{\sigma\sigma}$, naturally leads to the super-cell periodicity of the self-energy, $\Sigma(i, j; \mathrm{i}\omega_n)$, with respect to the super-cell translation vectors, $\mathbf{r}_{N_c}$. This provides us with the DCA [15] coarse graining of the self-energy in k-space for a general lattice structure. Note that in contrast to the original derivation of the DCA in k-space, our derivation is in real space. In the DCA it is not obvious why the Coulomb interaction where employed should be same as the original lattice model [19]. Furthermore we are not coarse graining the lattice band structure, in contrast to CDMFT [14].

This paper is organized in the following manner. In section 2 the model is introduced, then the equation of motion and its corresponding Dyson equation is derived for the next stages. In section 3 the EMSCA (generalized DCA) formalism is introduced. In section 4 the EMSCA is applied to a disordered system and the NLCPA [17] formalism is derived. Finally, in section 5, the EMSCA is applied to a disordered interacting system and a closed set of equations for performing numerical calculations is obtained.

2. Model

We start our investigation by studying a general tight binding model for an interacting alloy system, which is given by

$$H = -\sum_{ij\sigma\sigma'} t_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} \delta_{\sigma\sigma'} + \sum_{i\sigma} (\varepsilon_i - \mu)\hat{n}_{i\sigma} + \sum_{ij\sigma\sigma'} U_{ij}^{\sigma\sigma'} \hat{n}_{i\sigma}\hat{n}_{j\sigma'}, \tag{1}$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron with spin σ on lattice site i, $\hat{n}_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the number operator and $t_{ij}^{\sigma\sigma'}$ are the random hopping integrals between i and j lattice sites with spin σ and σ' respectively. μ is the chemical potential and ε_i is the random on-site energy, where it takes the values $-\delta/2$ with probability $1 - c$ for the host sites and $\delta/2$ with probability c for impurity sites. $U_{ij}^{\sigma\sigma'}$ is a positive or negative interaction potential between electrons on the lattice sites i and j.

The equation of motion for electrons corresponding to the above Hamiltonian, equation (1), is given by

$$\sum_{l\sigma''} \left(\left(\frac{\partial}{\partial\tau} - \varepsilon_i + \mu \right) \delta_{il}\delta_{\sigma\sigma''} - t_{il}^{\sigma\sigma''}\delta_{\sigma\sigma''} \right) G^{\sigma''\sigma'}(l\tau, j\tau') + \sum_{l\sigma''} U_{lj}^{\sigma\sigma''} G_2^{\sigma''\sigma'}(l\tau, l\tau, l\tau^{+}, j\tau') = \delta(\tau - \tau')\delta_{ij}\delta_{\sigma\sigma'} \tag{2}$$

where τ and τ' are imaginary time, $G^{\sigma\sigma'}(i\tau, j\tau')$ is the random interacting single particle Green function and $G_2^{\sigma\sigma'}(i\tau, i\tau, i\tau^{+}, j\tau')$ is the two particle Green function. The random hopping integrals, $t_{ij}^{\sigma\sigma}$, can be defined in terms of clean system hopping, $t_{ij}^{0\sigma\sigma}$, and the hopping integral deviations, $\delta t_{ij}^{\sigma\sigma}$, in a such way that the hopping randomness is included just in the $\delta t_{ij}^{\sigma\sigma}$, where

$$t_{ij}^{\sigma\sigma} = t_{ij}^{0\sigma\sigma} + \delta t_{ij}^{\sigma\sigma} \tag{3}$$

where just the second term on the right-hand side of equation (3) is random. The Dyson equation corresponding to equation (2) for the averaged Green function, $\bar{G}^{\sigma\sigma'}(l\tau'', j\tau')$, is [20]

$$\sum_{l\sigma''} \left(\left(\frac{\partial}{\partial\tau} - \varepsilon_i + \mu \right) \delta_{il}\delta_{\sigma\sigma''} - t_{il}^{0\sigma\sigma''}\delta_{\sigma\sigma''} \right) \bar{G}^{\sigma''\sigma'}(l\tau, j\tau') + \sum_{l\sigma''} \int \mathrm{d}\tau''\, \Sigma^{\sigma\sigma''}(i\tau, l\tau'')\bar{G}^{\sigma''\sigma'}(l\tau'', j\tau') = \delta(\tau - \tau')\delta_{ij}\delta_{\sigma\sigma'} \tag{4}$$

where the self-energy, $\Sigma^{\sigma\sigma'}(i\tau, l\tau')$, is defined by

$$\sum_{l\sigma''} \left\langle (\varepsilon_i\delta_{il}\delta_{\sigma\sigma''} + \delta t_{il}^{\sigma\sigma''}\delta_{\sigma\sigma''}) G^{\sigma''\sigma'}(l\tau, j\tau') + \sum_{l\sigma''} U_{lj}^{\sigma\sigma''} G_2^{\sigma''\sigma'}(l\tau, l\tau, l\tau^{+}, j\tau') \right\rangle = \sum_{l\sigma''} \int \mathrm{d}\tau''\, \Sigma^{\sigma\sigma''}(i\tau, l\tau'')\bar{G}^{\sigma''\sigma'}(l\tau'', j\tau'). \tag{5}$$

The imaginary time Fourier transform of equation (4) leads to

$$\sum_{l\sigma''} \left((\mathrm{i}\omega_n + \mu)\delta_{il}\delta_{\sigma\sigma''} - t_{il}^{0\sigma\sigma''}\delta_{\sigma\sigma''} - \Sigma^{\sigma\sigma''}(i, l; \mathrm{i}\omega_n) \right) \bar{G}^{\sigma''\sigma'}(l, j; \mathrm{i}\omega_n) = \delta_{ij}\delta_{\sigma\sigma'}, \tag{6}$$

where $\omega_n = \frac{1}{\beta}(2n + 1)\pi$ are the Matsubura frequencies. The space Fourier transform of the equation (6) is given by

$$\sum_{\sigma''} ((\mathrm{i}\omega_n + \mu)\delta_{\sigma\sigma''} - \epsilon_{\mathbf{k}}^{\sigma\sigma''}\delta_{\sigma\sigma''} - \Sigma^{\sigma\sigma''}(\mathbf{k}; \mathrm{i}\omega_n))\bar{G}^{\sigma''\sigma'}(\mathbf{k}; \mathrm{i}\omega_n) = \delta_{\sigma\sigma'}, \tag{7}$$

where the self-energy $\Sigma^{\sigma\sigma''}(\mathbf{k}; \mathrm{i}\omega_n)$ is defined by

$$\Sigma^{\sigma\sigma''}(\mathbf{k}; \mathrm{i}\omega_n) = \frac{1}{N}\sum_{i,j}\Sigma^{\sigma\sigma''}(i, j; \mathrm{i}\omega_n)\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}} \tag{8}$$

and also the clean system band structure, $\epsilon_{\mathbf{k}}^{\sigma\sigma''}$ is given by

$$\epsilon_{\mathbf{k}}^{\sigma\sigma} = \frac{1}{N}\sum_{i,j} t_{ij}^{0\sigma\sigma}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}}. \tag{9}$$

In the Fourier transformations of these equations the following orthogonality condition,

$$\frac{1}{N}\sum_{\mathbf{k}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}} = \delta_{ij} \tag{10}$$

is used, where the indices i and j run over all N lattice sites in the crystal.

The matrix form of equation (7) in the spinor space can be written as

$$\bar{\mathbf{G}}(\mathbf{k}; \mathrm{i}\omega_n) = ((\mathrm{i}\omega_n + \mu)\mathbf{I} - \boldsymbol{\epsilon}_{\mathbf{k}} - \boldsymbol{\Sigma}(\mathbf{k}; \mathrm{i}\omega_n))^{-1}, \tag{11}$$

where the band structure matrix, $\boldsymbol{\epsilon}_{\mathbf{k}}$, is

$$\boldsymbol{\epsilon}_{\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k}}^{\uparrow\uparrow} & 0 \\ 0 & \epsilon_{\mathbf{k}}^{\downarrow\downarrow} \end{pmatrix}, \tag{12}$$

the self-energy matrix $\boldsymbol{\Sigma}(\mathbf{k}; \mathrm{i}\omega_n)$ is given by

$$\boldsymbol{\Sigma}(\mathbf{k}; \mathrm{i}\omega_n) = \begin{pmatrix} \Sigma^{\uparrow\uparrow}(\mathbf{k}; \mathrm{i}\omega_n) & \Sigma^{\uparrow\downarrow}(\mathbf{k}; \mathrm{i}\omega_n) \\ \Sigma^{\downarrow\uparrow}(\mathbf{k}; \mathrm{i}\omega_n) & \Sigma^{\downarrow\downarrow}(\mathbf{k}; \mathrm{i}\omega_n) \end{pmatrix}, \tag{13}$$

and the average Green function matrix, $\mathbf{G}(\mathbf{k}; \mathrm{i}\omega_n)$, is defined by

$$\mathbf{G}(\mathbf{k}; \mathrm{i}\omega_n) = \begin{pmatrix} G^{\uparrow\uparrow}(\mathbf{k}; \mathrm{i}\omega_n) & G^{\uparrow\downarrow}(\mathbf{k}; \mathrm{i}\omega_n) \\ G^{\downarrow\uparrow}(\mathbf{k}; \mathrm{i}\omega_n) & G^{\downarrow\downarrow}(\mathbf{k}; \mathrm{i}\omega_n) \end{pmatrix}; \tag{14}$$

also, $\mathbf{I}$ is a 2×2 unit matrix. Hence the clean non-interacting Green function is given by

$$\mathbf{G}^0(\mathbf{k}; \mathrm{i}\omega_n) = ((\mathrm{i}\omega_n + \mu)\mathbf{I} - \boldsymbol{\epsilon}_{\mathbf{k}})^{-1}. \tag{15}$$

So, the real-space correspondence of equation (7) can be written as

$$\bar{\mathbf{G}}(i, j; \mathrm{i}\omega_n) = \mathbf{G}^0(i, j; \mathrm{i}\omega_n) + \sum_{ll'}\mathbf{G}^0(i, l; \mathrm{i}\omega_n)\boldsymbol{\Sigma}(l, l'; \mathrm{i}\omega_n)\bar{\mathbf{G}}(l', j; \mathrm{i}\omega_n), \tag{16}$$

where the real-space clean non-interacting Green function, $\mathbf{G}^0(i, j; \omega_n)$, is

$$\mathbf{G}^0(i, j; \mathrm{i}\omega_n) = \frac{1}{N}\sum_{\mathbf{k}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}}\mathbf{G}^0(\mathbf{k}; \mathrm{i}\omega_n), \tag{17}$$

and the average single particle Green function is defined by

$$\bar{\mathbf{G}}(i, j; \mathrm{i}\omega_n) = \frac{1}{N}\sum_{\mathbf{k}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{ij}}\bar{\mathbf{G}}(\mathbf{k}; \mathrm{i}\omega_n). \tag{18}$$

Equations (5) and (16) cannot be solved exactly. The single site approximations such as DMFT and CPA for the interacting and disordered systems are used to solve these equations [5, 6]. It is well known that in these approximations the inter-site effects have been neglected. Here our task is going beyond such single site approximations to preserve inter-site effects. In the next section we introduce our method (EMSCA) and we show that, for the case of $\delta t_{ll'}^{\sigma\sigma''} = 0$ and $U_{ll'}^{\sigma\sigma''} = 0$, it is equivalent to the NLCPA [17], and also that for the case of a clean interacting system it leads to a real-space derivation of the DCA [15] for a general lattice structure.

3. Effective medium super-cell approximation (EMSCA) or generalized DCA

Consider a random interacting system which is divided into similar volume super-cells where each super-cell includes N_c sites and has original lattice symmetry. The super-cell average Green function, corresponding to equation (16), is

$$\bar{\mathbf{G}}_{\rm sc}(I, J; \mathrm{i}\omega_n) = \mathbf{G}^0(I, J; \mathrm{i}\omega_n) + \sum_{ll'} \mathbf{G}^0(I, l; \mathrm{i}\omega_n)\boldsymbol{\Sigma}(l, l'; \mathrm{i}\omega_n)\bar{\mathbf{G}}_{\rm sc}(l', J; \mathrm{i}\omega_n), \tag{19}$$

where I and J refer to sites in the same super-cell and indices l, l' refer to the whole lattice sites. Now we apply an approximation (EMSCA) which is based on three assumptions: first, *neglecting interaction between electrons on different super-cells*, i.e.,

$$U_{ij}^{\sigma\sigma'} = 0, \qquad \text{if } i \text{ and } j \notin \text{ same super-cell}, \tag{20}$$

second, *neglecting hopping integral deviations*, $\delta t_{ij}^{\sigma\sigma}$, when i and j are in the different super-cells, i.e.,

$$\delta t_{ij}^{\sigma\sigma} = 0, \qquad \text{if } i \text{ and } j \notin \text{ same super-cell} \tag{21}$$

and finally, *neglecting disorder multiple scattering and also correlations between different super-cells*. Since in the averaged system the self-energy is due to interactions and disorder scattering, which includes impurity multiple scattering and interaction correlations, then by our assumption that there is no correlation and multiple scattering between different super-cells, we have

$$\boldsymbol{\Sigma}_{\rm sc}(i, j; \mathrm{i}\omega_n) = 0, \qquad \text{if } i \text{ and } j \notin \text{ same super-cell}. \tag{22}$$

Since in the averaged system we have all possible impurity configurations and interaction contributions with their own weights (probabilities) for each super-cell, so all super-cell self-energies should be the same. This means that the self-energies in each super-cell are independent of other super-cells and they are periodic with respect to the super-cell translation vectors, $\mathbf{r}_{N_c}$,

$$\boldsymbol{\Sigma}_{\rm sc}(\mathbf{r}_{IJ} + \mathbf{r}_{N_c}; \mathrm{i}\omega_n) = \boldsymbol{\Sigma}_{\rm sc}(\mathbf{r}_{IJ}; \mathrm{i}\omega_n), \tag{23}$$

where I and J refer to sites in the same super-cell and the super-cell translation vector $\mathbf{r}_{N_c}$ is given by

$$\mathbf{r}_{N_c} = \sum_{i=1}^{3} m_i\, N_{ci}\, \mathbf{a}_i, \tag{24}$$

where $N_c = N_{c1}\, N_{c2}\, N_{c3}$ is the number of lattice sites in a three-dimensional super-cell, $\mathbf{a}_i$ are primitive vectors of real lattice, N_{ci} is the number of sites in the super-cell in the ith direction and m_i are integers. Figure 1 shows $\mathbf{r}_{N_c}$ for a two-dimensional lattice with periodicity over nine sites in each super-cell. Note that when $N_c \to \infty$ all super-cells will be coincident and are equal to the full real lattice. Equation (20) leads to the super-cell periodicity for the interaction potential matrix, $\mathbf{U}_{\rm sc}(I, J)$, where

$$\mathbf{U}_{\rm sc}(I, J) = \begin{pmatrix} U_{\rm sc}^{\uparrow\uparrow}(I, J) & U_{\rm sc}^{\uparrow\downarrow}(I, J) \\ U_{\rm sc}^{\downarrow\uparrow}(I, J) & U_{\rm sc}^{\downarrow\downarrow}(I, J) \end{pmatrix}, \tag{25}$$

which is

$$\mathbf{U}_{\rm sc}(\mathbf{r}_{IJ} + \mathbf{r}_{N_c}) = \mathbf{U}_{\rm sc}(\mathbf{r}_{IJ}). \tag{26}$$

The Fourier transformation of equations (23) and (26) implies that

$$\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{N_c}} = 1. \tag{27}$$

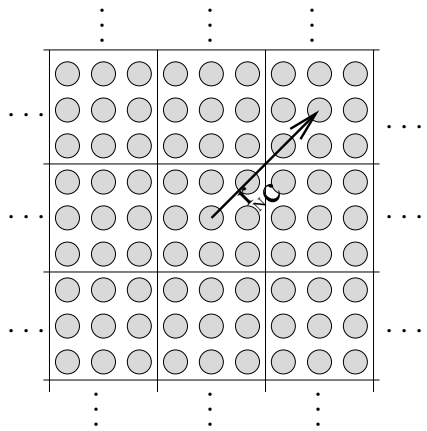

Figure 1. A two-dimensional lattice is divided into similar super-cells of nine sites where each super-cell has the original lattice symmetry. The arrow indicates the super-cell periodicity vector $\mathbf{r}_{N_c} = 3\mathbf{a}_1 + 3\mathbf{a}_2$, where $N_{c1} = 3$ and $N_{c2} = 3$.

Thus the wavevectors of the self-energy, $\mathbf{\Sigma}(\mathbf{k}; \mathrm{i}\omega_n)$, and the interaction potential, $\mathbf{U}(\mathbf{k})$, are restricted to the super-cell wavevectors $\mathbf{K}_n$ which are given by

$$\mathbf{K}_n = \sum_{i=1}^{3} \frac{n_i}{N_{ci}} \mathbf{b_i}, \tag{28}$$

where $\mathbf{b_i}$ are the reciprocal-lattice primitive vectors and n_i is an integer number. Note that in the limit of $N_{ci} \to N_i$ (where the super-cell is extended to the whole lattice) the super-cell wavevectors, $\mathbf{K}_n$, convert to the following allowed Bloch wavevectors [21],

$$\mathbf{k} = \sum_{i=1}^{3} \frac{n_i}{N_i} \mathbf{b_i}. \tag{29}$$

Since the set of $\{\mathbf{K}_n\}$ vectors divides the volume of the first Brillouin zone into N_c equal patches, following the DCA method, we identify the nth patch by its corresponding wavevector $\mathbf{K}_n$ that is located at its centre. Therefore we define the relation between $\mathbf{K}_n$ and $\mathbf{k}$ inside each patch as follows:

$$\mathbf{k} = \mathbf{K}_n + \mathbf{k}'_n \tag{30}$$

where $\mathbf{k}'_n$ are the wavevectors inside the nth patch with respect to the centre of the patch. Figure 2 illustrates the FBZ of a two-dimensional square lattice and the patches where they correspond to the nine sites of the EMSCA. For one of the patches, the relationships between $\mathbf{k}$, $\mathbf{k}'$ and the super-cell wavevectors $\mathbf{K}_n$ are shown schematically.

Therefore, by inserting equations (28) and (22) into (8) we found that

$$\mathbf{\Sigma}_{\mathrm{sc}}(\mathbf{K}_n; \mathrm{i}\omega_n) = \frac{1}{N_c} \sum_{I,J} \mathrm{e}^{\mathrm{i}\mathbf{K}_n \cdot \mathbf{r}_{IJ}} \mathbf{\Sigma}_{\mathrm{sc}}(I, J; \mathrm{i}\omega_n). \tag{31}$$

Also, by applying the EMSCA conditions, equations (20) and (27), to the following exact relation,

$$\mathbf{U}(\mathbf{k}) = \frac{1}{N} \sum_{i,j} \mathbf{U}(i, j) \mathrm{e}^{\mathrm{i}\mathbf{k} \cdot \mathbf{r}_{ij}}, \tag{32}$$

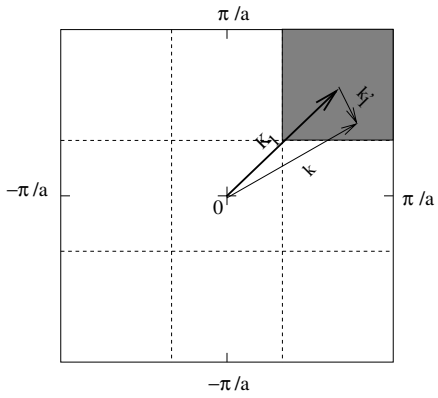

Figure 2. Relation between $\mathbf{k}$, $\mathbf{K}_n$ and $\mathbf{k}'_n$ in the first Brillouin zone (FBZ) for a two-dimensional system with a nine-site super-cell. As given by equations (28) and (30) there are nine different $\mathbf{K}_n$ in the FBZ, and so the FBZ is divided into nine equal areas, while each $\mathbf{K}_n$ is located at the centre of one of these areas. Each sub-zone should have the FBZ symmetry.

we found a similar coarse graining for the interaction potential,

$$\mathbf{U}(\mathbf{K}_n) = \frac{1}{N_c}\sum_{I,J}\mathbf{U}_{\rm sc}(I,J)\mathrm{e}^{\mathrm{i}\mathbf{K}_n\cdot\mathbf{r}_{IJ}}. \tag{33}$$

The inverse Fourier transformation of the self-energy, $\mathbf{\Sigma}(\mathbf{K}_n;\mathrm{i}\omega_n)$, to the real super-cell is

$$\mathbf{\Sigma}_{\rm sc}(I,J;\mathrm{i}\omega_n) = \frac{1}{N_c}\sum_{\mathbf{K}_n}\mathrm{e}^{-\mathrm{i}\mathbf{K}_n\cdot\mathbf{r}_{IJ}}\mathbf{\Sigma}(\mathbf{K}_n;\mathrm{i}\omega_n), \tag{34}$$

and similarly for $\mathbf{U}(\mathbf{K}_n)$ it is

$$\mathbf{U}_{\rm sc}(I,J) = \frac{1}{N_c}\sum_{\mathbf{K}_n}\mathbf{U}(\mathbf{K}_n)\mathrm{e}^{-\mathrm{i}\mathbf{K}_n\cdot\mathbf{r}_{IJ}}, \tag{35}$$

where the orthogonality condition in a super-cell is given by

$$\frac{1}{N_c}\sum_{\mathbf{K}_n}\mathrm{e}^{-\mathrm{i}\mathbf{K}_n\cdot\mathbf{r}_{IJ}} = \delta_{IJ}. \tag{36}$$

By comparing equations (36) and (10) we find that the super-cell approximation is equivalent to the replacement

$$\mathrm{e}^{\mathrm{i}\mathbf{k}'_n\cdot\mathbf{r}_{IJ}} \approx 1. \tag{37}$$

Now by inserting equations (37), (31) and (27) into (18), the super-cell average Green function, $\bar{\mathbf{G}}_{\rm sc}(I,J;\mathrm{i}\omega_n)$, is given by,

$$\bar{\mathbf{G}}_{\rm sc}(I,J;\mathrm{i}\omega_n) = \frac{1}{N_c}\sum_{\mathbf{K}_n}\mathrm{e}^{\mathrm{i}\mathbf{K}_n\cdot\mathbf{r}_{IJ}}\bar{\mathbf{G}}(\mathbf{K}_n;\mathrm{i}\omega_n), \tag{38}$$

where

$$\bar{\mathbf{G}}(\mathbf{K}_n;\mathrm{i}\omega_n) = \frac{N_c}{N}\sum_{\mathbf{k}'_n}\left(\mathbf{G}^0(\mathbf{K}_n+\mathbf{k}'_n;\mathrm{i}\omega_n)^{-1} - \Sigma(\mathbf{K}_n;\mathrm{i}\omega)\right)^{-1}. \tag{39}$$

By applying the DCA condition [15, 16, 22], $N_c = L^D$, in k-space where the coarse grained wavevectors are chosen as $K_\alpha = \frac{2\pi}{L}$, a relation similar to equation (27) is introduced [15, 22].

Since the super-cell should have the original lattice symmetry and the DCA condition gives us a super-cell with equal sides, so the DCA condition, $N_c = L^D$, is not applicable for other lattice structures and cannot give us a recipe for providing $\mathbf{K}_n$, while in our method each super-cell has the complete symmetry of the real lattice and hence its corresponding sub-zone (coarse grained zone) in the FBZ has the FBZ symmetry. Therefore according to our EMSCA formalism one can easily find $\mathbf{K}_n$ for a general lattice structure [18].

In order to obtain $\bar{\mathbf{G}}_{\rm sc}(I, J; \mathrm{i}\omega_n)$ from equation (38), we should have $\mathbf{\Sigma}_{\rm sc}(I, J; \mathrm{i}\omega_n)$, for which it is needed to have other equations to complete the self-consistency loop. These equations are obtained by applying the EMSCA to the system partition function as follows. The partition function of the system with the Hamiltonian equation (1) is given by

$$Z = \langle \mathrm{Tr}\, \mathrm{e}^{-\beta \hat{H}} \rangle_r, \tag{40}$$

where $\langle\,\rangle_r$ denotes the configurational average over random energies ε_i and $\delta t_{ij}^{\sigma\sigma}$. The partition function, equation (40), can be rewritten as [23]

$$Z = \left\langle \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \mathrm{e}^{-S} \right\rangle_r, \tag{41}$$

where the action S is

$$S = \sum_{ij\sigma\sigma'} \int_0^\beta \mathrm{d}\tau\, \bar{\psi}_{i\sigma}\delta_{\sigma\sigma'}\left(\delta_{ij}\left(\frac{\partial}{\partial\tau} - \mu\right) + t_{ij}^{0\sigma\sigma'}\right)\psi_{j\sigma}(\tau) + S_{\rm r-i}, \tag{42}$$

and $S_{\rm r-i}$ is

$$S_{\rm r-i} = \sum_{ij\sigma\sigma'} \int \mathrm{d}\tau\, \bar{\psi}_{i\sigma}\psi_{i\sigma}U_{ij}^{\sigma\sigma'}\bar{\psi}_{j\sigma'}(\tau)\psi_{j\sigma'}(\tau) + \sum_{ij\sigma} \int \mathrm{d}\tau\, \bar{\psi}_{i\sigma}(\tau)\varepsilon_i\delta_{ij}\psi_{j\sigma}(\tau) \tag{43}$$

$$+ \sum_{ij\sigma\sigma'} \int \mathrm{d}\tau \bar{\psi}_{i\sigma}(\tau)\delta_{\sigma\sigma'}\delta t_{ij}^{\sigma\sigma'}\psi_{j\sigma'}(\tau), \tag{44}$$

in which $\mathcal{D}\Psi = \Pi_i\, \mathrm{d}\psi_{i\sigma}\, \mathrm{d}\psi_{i\sigma}$ and $\mathcal{D}\bar{\Psi} = \Pi_i\, \mathrm{d}\bar{\psi}_{i\sigma}\, \mathrm{d}\bar{\psi}_{i\sigma}$, where $\mathrm{d}\bar{\psi}_{i\sigma} = \lim_{M\to\infty} \Pi_{m=1}^M \mathrm{d}\bar{\psi}_{i\sigma}(\tau_m)$, $\mathrm{d}\psi_{i\sigma} = \lim_{M\to\infty} \Pi_{m=1}^M \mathrm{d}\psi_{i\sigma}(\tau_m)$. Equation (42) can be rewritten as

$$S = \int_0^\beta \mathrm{d}\tau\, \mathrm{d}\tau' \sum_{ij\sigma\sigma'} \bar{\psi}_{i\sigma}(\tau)(\mathbf{G}^{0^{-1}})_{ij\sigma\sigma'}\psi_{j\sigma'}(\tau') + S_{\rm r-i}, \tag{45}$$

where

$$\begin{aligned}
&\delta_{\sigma\sigma'}\left(\delta_{ij}\left(\frac{\partial}{\partial\tau} - \mu\right) + t_{ij}^{0\sigma\sigma'}\right)\psi_{j\sigma'}(\tau) \\
&\quad = \int_0^\beta \mathrm{d}\tau' \frac{1}{\beta}\sum_{\omega_n} \delta_{\sigma\sigma'}\left(\delta_{ij}(\mathrm{i}\omega_n - \mu) + t_{ij}^{0\sigma\sigma'}\right)\mathrm{e}^{\mathrm{i}\omega_n(\tau-\tau')}\psi_{j\sigma}(\tau') \\
&\quad = \int_0^\beta \mathrm{d}\tau'\, (\mathbf{G}^{0^{-1}})_{ij\sigma\sigma'}(\tau - \tau')\psi_{j\sigma'}(\tau'),
\end{aligned} \tag{46}$$

and the clean non-interacting Green function matrix, $\mathbf{G}^0(\mathrm{i}\omega_n)$, is defined by

$$(\mathbf{G}^{0^{-1}})_{ij\sigma\sigma'}(\tau - \tau') = \frac{\delta_{\sigma\sigma'}}{\beta}\sum_{\omega_n}\left(\delta_{ij}(\mathrm{i}\omega_n - \mu) + t_{ij}^{0\sigma\sigma'}\right)\mathrm{e}^{\mathrm{i}\omega_n(\tau-\tau')}. \tag{47}$$

By use of equation (16) the clean Green function, $\mathbf{G}^0$, can be expressed in terms of the average Green function, $\bar{\mathbf{G}}$, and self-energy, $\mathbf{\Sigma}$, as

$$\mathbf{G}^{0^{-1}} = \bar{\mathbf{G}}^{-1} + \mathbf{\Sigma}. \tag{48}$$

By inserting equation (48) into (45), we have

$$S = \int \mathrm{d}\tau\, \mathrm{d}\tau' \sum_{ij\sigma\sigma'} \bar{\psi}_{i\sigma}(\tau) \left(\bar{\mathbf{G}}^{-1}\right)_{ij\sigma\sigma'} \psi_{j\sigma'}(\tau') + S_{\mathrm{r-i-s}}, \tag{49}$$

where

$$\begin{aligned} S_{\mathrm{r-i-s}} = & \sum_{ij\sigma\sigma'} \int \mathrm{d}\tau\, \bar{\psi}_{i\sigma}\psi_{i\sigma} U_{ij}^{\sigma\sigma'} \bar{\psi}_{j\sigma'}(\tau)\psi_{j\sigma'}(\tau) \\ & + \sum_{ij\sigma\sigma'} \int \mathrm{d}\tau\, \mathrm{d}\tau'\, \bar{\psi}_{i\sigma}(\tau)\delta_{\sigma\sigma'}(\varepsilon_i\delta_{ij} + \delta t_{ij}^{\sigma\sigma'})\psi_{j\sigma'}(\tau) \\ & - \sum_{ij\sigma\sigma'} \int \mathrm{d}\tau'\, \mathrm{d}\tau\, \bar{\psi}_{i\sigma}(\tau)\mathbf{\Sigma}_{ij}^{\sigma\sigma'}(\tau - \tau')\psi_{j\sigma}(\tau'). \end{aligned} \tag{50}$$

Now we apply the EMSCA, in which we take an average over all super-cells except one super-cell which is denoted by $\{IJ\}$. In equation (50) this is equivalent to replacing $U_{ij}^{\sigma\sigma'} + \delta_{\sigma\sigma'}(\varepsilon_i\delta_{ij} + \delta t_{ij}^{\sigma\sigma'})$ by $\mathbf{\Sigma}_{ij}^{\sigma\sigma'}(\tau - \tau')$ when i and $j \notin \{IJ\}$. Hence equation (41) converts to

$$Z_{\mathrm{EMSCA}} = Z_{\mathrm{sc}} \int \Pi_{i\notin\{I\},\sigma} \left(\mathrm{d}\bar{\psi}_{i\sigma}\, \mathrm{d}\psi_{i\sigma}\right) \mathrm{e}^{-\int \mathrm{d}\tau\, \mathrm{d}\tau' \sum_{\sigma\sigma'} \sum_{ij\notin\{I,J\}} \bar{\psi}_{i\sigma}(\tau)\left(\bar{\mathbf{G}}^{-1}\right)_{ij\sigma\sigma'}\psi_{j\sigma'}(\tau')}, \tag{51}$$

where the super-cell partition function, Z_{sc}, is given by

$$Z_{\mathrm{sc}} = \left\langle \int \Pi_{I=1}^{N_c,\sigma} \left(\mathrm{d}\bar{\psi}_{I\sigma}\, \mathrm{d}\psi_{I\sigma}\right) \mathrm{e}^{-S_{\mathrm{r-i}}^{\mathrm{sc}}} \right\rangle_{\mathrm{r-sc}} \tag{52}$$

and the super-cell action in the effective medium, $S_{\mathrm{r-i}}^{\mathrm{sc}}$, is

$$\begin{aligned} S_{\mathrm{r-i}}^{\mathrm{sc}} = & \sum_{IJ\sigma\sigma'} \int \mathrm{d}\tau\, \mathrm{d}\tau'\, \bar{\psi}_{I\sigma}(\tau) \left(\mathcal{G}^{-1}\right)_{IJ\sigma\sigma'}(\tau - \tau')\psi_{J\sigma'}(\tau') \\ & - \sum_{IJ\sigma\sigma'} \int \mathrm{d}\tau\, \bar{\psi}_{I\sigma}\psi_{I\sigma} U_{scIJ}^{\sigma\sigma'} \bar{\psi}_{J\sigma'}(\tau)\psi_{J\sigma'}(\tau) \\ & + \sum_{IJ\sigma\sigma'} \int \mathrm{d}\tau\, \bar{\psi}_{I\sigma}(\tau)\delta_{\sigma\sigma'}(\varepsilon_I\delta_{IJ} + \delta t_{IJ}^{\sigma\sigma'})\psi_{J\sigma'}(\tau), \end{aligned} \tag{53}$$

in which the super-cell cavity Green function matrix, $\mathcal{G}$, is defined by

$$\mathcal{G}^{-1} = \bar{\mathbf{G}}_{\mathrm{sc}}^{-1} - \mathbf{\Sigma}_{\mathrm{sc}}. \tag{54}$$

The matrix element of equation (54) is given by the following Dyson-like equation for the super-cell sites,

$$\bar{G}_{\mathrm{sc}}(I, J; \mathrm{i}\omega_n) = \mathcal{G}(I, J; \mathrm{i}\omega_n) + \sum_{L,L'} \mathcal{G}(I, L; \mathrm{i}\omega_n)\Sigma_{\mathrm{sc}}(L, L'; \mathrm{i}\omega_n)\bar{G}_{\mathrm{sc}}(L', J; \mathrm{i}\omega_n). \tag{55}$$

The second part of the right-hand side of equation (51) is the super-cell excluded effective medium partition function which is easily integrable, due to bi-linearity of the Grassmann variables, $\bar{\psi}_{I\sigma}(\tau)$ and $\psi_{I\sigma}(\tau)$. But the partition function of the super-cell, Z_{sc}, where it is embedded in an effective medium environment, is not integrable directly due to four point Grassmann variables in its integrand. Many approximations, such as the Hartree–Fock approximation, quantum Monte Carlo approximation, could be used to decouple the four point Grassmann variables to two point variables. To see the advantages of the static version of the EMSCA method with respect to the CPA, first we investigate a disordered system without interaction between electrons ($U_{scIJ}^{\sigma\sigma'}$). Note that in equation (54) both the super-cell cavity Green function $\mathcal{G}$ and super-cell average Green function $\bar{\mathbf{G}}$ are causal; hence the super-cell self-energy $\mathbf{\Sigma}$ is casual.

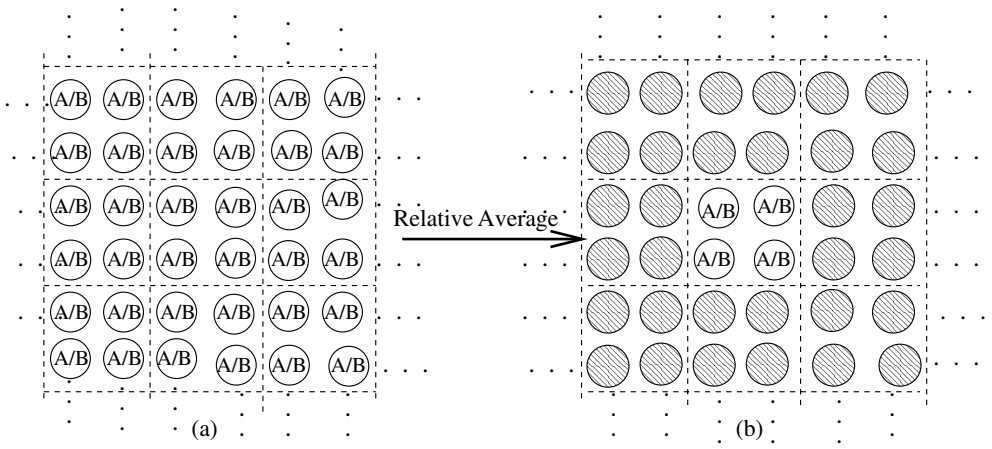

Figure 3. A four site impurity super-cell, $N_c = 4$, in an effective medium of mean-field super-cells.

4. Static EMSCA for a disordered system

For a disordered system where $U_{scIJ}^{\sigma\sigma'} = 0$, equations (52) and (53) lead to

$$\mathbf{G}_{\rm sc}^{\rm imp\,-1}(\tau - \tau') = \mathcal{G}(\mathrm{i}\omega_n)^{-1}(\tau - \tau') - \delta(\tau - \tau')\varepsilon^{\rm sc}, \tag{56}$$

where $\varepsilon_{\rm sc}$ is the super-cell impurity matrix, where its matrix elements are given by

$$\varepsilon_{IJ}^{\rm sc} = (\varepsilon_I \delta_{IJ} + \delta t_{IJ}^{\sigma\sigma'})\delta_{\sigma\sigma'}. \tag{57}$$

The imaginary-time Fourier transform of equation (56) implies that

$$\mathbf{G}_{\rm sc}^{\rm imp}(\mathrm{i}\omega_n)^{-1} = \mathcal{G}(\mathrm{i}\omega_n)^{-1} - \varepsilon^{\rm sc}, \tag{58}$$

where the matrix element of equation (58) can be written as

$$G_{\rm sc}^{\rm imp}(I, J, \mathrm{i}\omega_n) = \mathcal{G}(I, J, \mathrm{i}\omega_n) + \sum_{LL'} \mathcal{G}(I, L, \mathrm{i}\omega_n)\varepsilon_{LL'}^{\rm sc} G_{\rm sc}^{\rm imp}(L', J, \mathrm{i}\omega_n). \tag{59}$$

The average of the impurity Green function $G_{\rm sc}^{\rm imp}(I, J; \mathrm{i}\omega_n)$ over all impurity configurations $\{\varepsilon_{IJ}^{\rm sc}\}$ in the super-cell is given by

$$\langle G_{\rm sc}^{\rm imp}(I, J; \mathrm{i}\omega_n)\rangle = \bar{G}_{\rm sc}(I, J; \mathrm{i}\omega_n). \tag{60}$$

For a disordered system, equations (38), (55), (59) and (60) construct a closed set of equations that should be solved self-consistently.

Figure 3 shows an example of a four site super-cell impurity, $N_c = 4$, that is embedded in an effective medium where the average has been taken over all super-cells except the *impurity super-cell*. The above system of equations can be implemented numerically by the following algorithm.

(1) Make a guess for $\Sigma(\mathbf{K}_n; E)$, usually zero.
(2) Calculate $\bar{G}(\mathbf{K}_n; E)$ from equation (39).
(3) Use equation (55) to calculate the Fourier transform of the cavity Green function

$$\mathcal{G}(\mathbf{K}_n; E) = (\bar{G}^{-1}(\mathbf{K}_n; E) + \Sigma_{\rm sc}(\mathbf{K}_n; E))^{-1}. \tag{61}$$

(4) Calculate the impurity super-cell Green function $G_{\rm sc}^{\rm imp}(I, J; E)$ from equation (58).

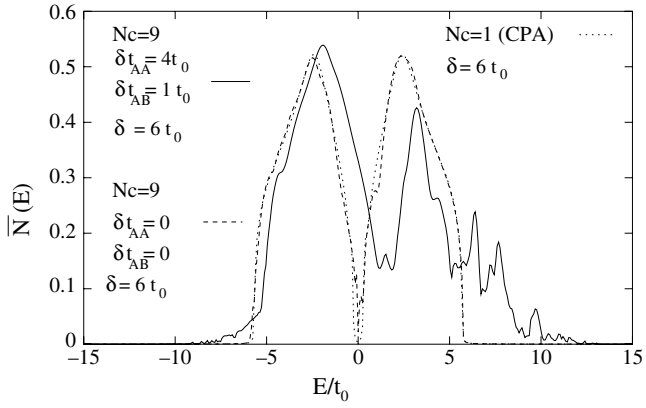

Figure 4. The density of states of a two-dimensional square lattice of a binary alloy A_cB_{1-c} at half band filling, $\bar{n} = 1$, for $c = 0.5$ and $\delta = 6t^0$ when $N_c = 1$ (CPA) and $N_c = 9$. We compared the $N_c = 1$ density of states with two cases of $N_c = 9$, first $\delta t_{\mathrm{AA}} = 0$, $\delta t_{\mathrm{AB}} = 0$ and second $\delta t_{\mathrm{AA}} = 4t^0$, $\delta t_{\mathrm{AB}} = t^0$. For both non-hopping integral randomness cases band splitting occurred (a metal–insulator phase transition took place), while for the other it did not (it still is a metal).

(5) Calculate the average Green function from equation (60) and Fourier transform it to the super-cell wavevector $\mathbf{K}_n$ space by using equation (36).
(6) Using equation (61) calculate the new self-energies $\Sigma_{\mathrm{sc}}(\mathbf{K}_n; E)$, go back to step 1 and repeat the whole process until convergence has been obtained to a desired accuracy.

As an application of this method we calculate the density of states of a two-dimensional square lattice at half band filling, $\bar{n} = 1$ and $\delta = 6t^0$ (where $t^0_{\langle ij\rangle} = t^0$ are the clean system nearest neighbours hopping integrals) in which $N_c = 1$ (CPA) and $N_c = 9$. We assume that the hopping integrals for both spin up and down are the same, $t^{\sigma\sigma}_{ij} = t_{ij}$. For the case of $N_c = 9$, we also show the effects of introducing random hopping parameters, by considering the two cases $\delta t_{\mathrm{AA}} = 0$, $\delta t_{\mathrm{AB}} = 0$ and $\delta t_{\mathrm{AA}} = 4t^0$, $\delta t_{\mathrm{AB}} = t^0$, where

$$\delta t_{\langle ij\rangle} = t_{\mathrm{AA}} - t^0, \tag{62}$$

in which i and j are nearest neighbour sites and both are A type, and we also define

$$\delta t_{\langle ij\rangle} = t_{\mathrm{AB}} - t^0, \tag{63}$$

where at the nearest neighbour sites i and j, atoms of type A and B are located respectively. Figure 4 shows that for the $N_c = 1$ (CPA) and the case of $N_c = 9$ without random hopping, in which $\delta = 6t^0$, we are at the band splitting regime [24, 25]. In this case at half band filling a metal–insulator phase transition is taking place, in spite of the different gap sizes. However, for the case of $N_c = 9$ with random hopping $\delta t_{\mathrm{AA}} = 4t^0$, $\delta t_{\mathrm{AB}} = t^0$, band splitting does not take place, and thus the system is a metal. Therefore due to including randomness in both the on-site energies and the hopping integrals, the EMSCA technique can provide more realistic results.

5. EMSCA for a disordered interacting system

In the general case, to calculate the super-cell partition function, Z_{sc}, where both interaction and randomness are included it is possible to use the Hirsch–Hubbard–Stratonovich transformation (HHST) [26] to decouple the interaction term and map the interaction term to an auxiliary

Ising field. Although our method is general with respect to the interaction potential and randomness, for simplicity we concentrate our discussion on a repulsive on-site potential, $U_{ij}^{\sigma\sigma'} = U\delta_{ij}\delta_{\sigma,-\sigma}$. The HHST procedure is as follows. Divide the imaginary time interval, $[0, \beta]$, into M subintervals, $\Delta\tau = \frac{\beta}{M}$; hence the imaginary time at the lth slice is given by $\tau_l = l\frac{\beta}{M}$. Therefore the discretizing of imaginary times leads to $\int_0^\beta \mathrm{d}\tau = \sum_l \Delta\tau$, see for example [27], thus,

$$Z_{\mathrm{sc}} = \left\langle \int \Pi_\sigma \Pi_{I=1}^{N_c} \left(\mathrm{d}\bar{\psi}_{I\sigma}\, \mathrm{d}\psi_{I\sigma} \sum_{\{s_{I=\pm1}\}} \right) \mathrm{e}^{-S_{\mathrm{r-i}}^{\mathrm{sc}}} \right\rangle_{\mathrm{r-sc}}, \tag{64}$$

where the super-cell action $S_{\mathrm{r-i}}^{\mathrm{sc}}$ is

$$S_{\mathrm{r-i}}^{\mathrm{sc}} = (\Delta\tau)^2 \sum_{IJll'\sigma} \bar{\psi}_{I\sigma}(\tau_l) \times \left((\mathcal{G}^{-1})_{IJll'} + \left(\delta t_{IJ}^{\sigma\sigma} + \delta_{IJ} \left(\frac{\lambda\sigma s_{Il}}{(\Delta\tau)^2} - \frac{\varepsilon_I}{\Delta\tau} + \frac{U}{2\Delta\tau} \right) \right) \delta_{ll'+1} \right) \psi_{J\sigma}(\tau_{l'}). \tag{65}$$

We define the cluster impurity Green function $\mathbf{G}_{\mathrm{sc}}^{\mathrm{imp}}$ as

$$(\mathbf{G}_{\mathrm{sc}}^{\mathrm{imp}\,-1})_{IJll'} = (\mathcal{G}^{-1})_{IJll'} + \left(\delta t_{IJ}^{\sigma\sigma} + \delta_{IJ} \left(\frac{\lambda\sigma s_{Il}}{(\Delta\tau)^2} - \frac{\varepsilon_I}{\Delta\tau} + \frac{U}{2\Delta\tau} \right) \right) \delta_{ll'+1}. \tag{66}$$

By the DCA + QMC method [28] for just interacting systems an equation similar to equation (66) is found. The average of the impurity Green function, $\mathbf{G}_{\mathrm{sc}}^{\mathrm{imp}}$, over Ising fields and also impurity configurations is the super-cell effective average Green function $\bar{\mathbf{G}}_{\mathrm{sc}}(I, J; \tau_l, \tau_{l'})$, where is given by

$$\langle \mathbf{G}_{\mathrm{sc}}^{\mathrm{imp}}(I, J; \tau_l, \tau_{l'}) \rangle = \bar{\mathbf{G}}_{\mathrm{sc}}(I, J; \tau_l, \tau_{l'}). \tag{67}$$

The Fourier transform of equation (67) is

$$\bar{\mathbf{G}}_{\mathrm{sc}}(K_n; \mathrm{i}\omega_n) = \frac{1}{N_c} \sum_{ll'} \sum_{IJ} \mathrm{e}^{\mathrm{i}\mathbf{K}_n \cdot \mathbf{r}_{IJ}} \mathrm{e}^{\mathrm{i}\omega_n(\tau_l - \tau_{l'})} \bar{\mathbf{G}}_{\mathrm{sc}}(I, J; \tau_l, \tau_{l'}). \tag{68}$$

Equations (39), (55), (66)–(68) construct a closed set of equations that should be solved self-consistently.

The algorithm for the numerical process is as follows.

(1) Make a guess for the initial cluster self-energy, $\boldsymbol{\Sigma}(K_n; \mathrm{i}\omega)$, usually zero.
(2) From equation (39) calculate the cluster Green function, $\mathbf{G}(K_n; \mathrm{i}\omega)$.
(3) Calculate the cavity Green function $\boldsymbol{\mathcal{G}}(\mathbf{K}_n; \mathrm{i}\omega)$ from the Fourier transform of equation (55), $\boldsymbol{\mathcal{G}}^{-1}(\mathbf{K}_n; \mathrm{i}\omega_n) = \mathbf{G}^{-1}(\mathbf{K}_n; \mathrm{i}\omega_n) + \boldsymbol{\Sigma}(\mathbf{K}_n; \mathrm{i}\omega_n)$.
(4) Calculate the Fourier transform of the cavity Green function,

$$\mathcal{G}(I, J; \tau_l - \tau_{l'}) = \frac{1}{\beta N_c} \sum_n \sum_{\mathbf{K}_n} \mathcal{G}(\mathbf{K}_n; \mathrm{i}\omega_n) \mathrm{e}^{\mathrm{i}\omega_n(\tau_l - \tau_{l'})} \mathrm{e}^{-\mathrm{i}\mathbf{K}_n \cdot \mathbf{r}_{IJ}}. \tag{69}$$

(5) Calculate the new cluster Green function $\bar{\mathbf{G}}(I, J; \tau_l - \tau_{l'})$ from equations (66)–(68).
(6) Calculate the inverse Fourier transform of $\bar{\mathbf{G}}(I, J; \tau_l - \tau_{l'})$.
(7) Calculate the new self-energy $\boldsymbol{\Sigma}(\mathbf{K}_n; \mathrm{i}\omega_n)$ from

$$\boldsymbol{\Sigma}(\mathbf{K}_n; \mathrm{i}\omega_n) = \boldsymbol{\mathcal{G}}^{-1}(\mathbf{K}_n; \mathrm{i}\omega_n) - \mathbf{G}^{-1}(\mathbf{K}_n; \mathrm{i}\omega_n). \tag{70}$$

(8) Go to step 2 and repeat the whole process until it converges.

As an application, the EMSCA method is applied to a two-dimensional interacting binary alloy. Figure 5 shows the average density of states for the two different cases $U = 0$ and $2t^0$ where $\bar{n} = 1$, $c = 0.5$, $\delta = 2t^0$, $\delta t_{\mathrm{AA}} = 2t^0$ and $\delta t_{\mathrm{AB}} = t^0$. In the interaction case band splitting is taking place while for the non-interacting case it is not.

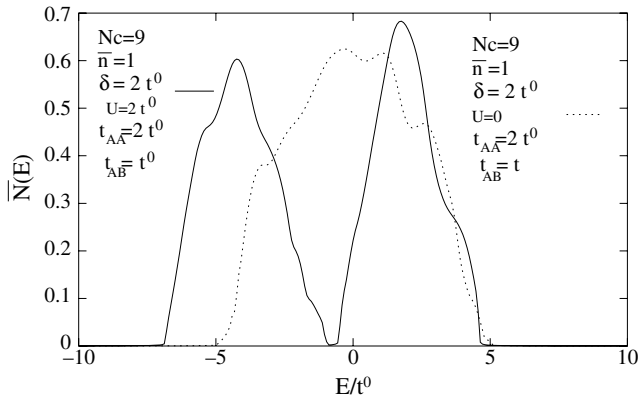

Figure 5. The nine-sites ($N_c = 9$) average density of states of a two-dimensional square lattice of an interacting binary alloy $A_c B_{1-c}$ at half band filling, $\bar{n} = 1$, for $c = 0.5$, $\delta = 2t^0$, $\delta t_{\mathrm{AA}} = 2t^0$ and $\delta t_{\mathrm{AB}} = t^0$ when $U = 0$ and $U = 2t^0$. Our results show that Coulomb interaction could lead to band splitting at high interaction potential strength.

6. Conclusions

We have introduced a real-space effective medium super-cell approximation (EMSCA) for random interacting systems which is equivalent to the generalized DCA including interactions and randomness in both hopping integrals and on-site energies simultaneously for a general lattice structure. This method is causal and preserves translational symmetry. For the case of $N_c = 1$, the EMSCA recovers both single site approximations, DMFT and CPA formalisms. However, for larger values of N_c the method simultaneously extends the CPA and DMFT by including the effects of impurity multiple scattering, allowing randomness in the hopping integrals and by inter-site correlations due to inter-site interactions. Furthermore, in the limit of $N_c \to \infty$ the method is exact. The EMSCA in the special case where hopping randomness is neglected, $\delta t_{IJ}^{\sigma\sigma} = 0$ and $U_{IJ}^{\sigma\sigma'} = 0$, leads to an alternative derivation of the NLCPA [17] technique for disordered systems. This derivation completely establishes the NLCPA as a valid and useful extension of the old and popular CPA method, which incorporates the effects of inter-site correlations. We showed that the periodicity of the super-cell self-energies $\Sigma_{\mathrm{sc}}(I, J; E)$ with respect to the super-cell translation vector $\mathbf{r}_{N_c}$ leads to the coarse graining of the self-energies in k-space and hence the average Green function. Then by applying the effective medium theory on the system partition function, we find two equations which relate the super-cell impurity Green function, $\mathbf{G}_{\mathrm{sc}}^{\mathrm{imp}}(I, J; \mathrm{i}\omega_n)$, and super-cell average Green function, $\bar{\mathbf{G}}_{\mathrm{sc}}(I, J; \mathrm{i}\omega_n)$, to the super-cell cavity Green function, $\mathcal{G}(I, J; \mathrm{i}\omega_n)$. This completes the whole formalism of a real-space method for disordered interacting systems as a generalization of the DCA to incorporate randomness in both hopping integrals and on-site energies simultaneously for a general lattice structure. In the especial case of an interacting system our formalism leads to a real-space derivation of the original DCA [15] for a general lattice structure.

Acknowledgments

I would like to thanks James F Annett and B L Györffy for helpful discussions.

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