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Cluster coherent potential approximation for the electronic structure of disordered alloys

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Abstract

We extend the single-site coherent potential approximation (CPA) to include the effects of non-local disorder correlations (alloy short-range order) on the electronic structure of random alloy systems. This is achieved by mapping the original Anderson disorder problem to that of a self-consistently embedded cluster. This cluster problem is then solved using the equations of motion technique. The CPA is recovered for cluster size $N_c = 1$. Various new features, compared to those observed in CPA, and related to repeated scattering on pairs of sites, reflecting the effect of short-range order are clearly visible in the density of states. It is explicitly shown that the cluster-CPA method always yields a positive-definite density of states. Anderson localization effects have been investigated within this approach. In general, we find that Anderson localization sets in before band splitting occurs, and that increasing partial order drives a continuous transition from an Anderson insulator to an incoherent metal.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The problem of atomic short-range order (SRO) and its effect on the character of electronic dynamics has been studied for many years now. It is relevant to the detailed understanding of the conditions under which a transition from metallic to an Anderson localized (AL), disordered insulator occurs with increasing disorder strength [1]. In the $d = \infty$ limit, the well-known coherent potential approximation (CPA) [2] provides the *exact* solution of this Anderson disorder problem. However, by construction, the CPA cannot access the specific effects (quantum interference from short-range scattering potentials) leading to AL behaviour. Such an endeavour demands explicit incorporation of the *dynamical* effect of SRO on carrier propagation in a disordered system, and thus, a cluster generalization of the CPA. Such attempts have indeed been carried out [3, 4], but are extremely cumbersome numerically. Additionally,

they do not always guarantee the correct analyticity properties of the Green functions: the few which do succeed in this respect, like the travelling cluster approximation (TCA) [4] and the dynamical cluster approximation (DCA) [5] are extremely tedious technically. Further, the study of the effects of SRO on carrier dynamics has, to our best knowledge, never been attempted using these approaches. It is obvious that attempting to tackle the harder problem of atomic (or doping-induced) SRO along with arbitrarily strong local electronic correlations, not to mention important aspects like the multi-orbital character of realistic transition metal-based oxide systems, with these approaches would be extremely numerically time-consuming. Given this, it is imperative to develop semi-analytical routes as far as possible, resulting in much better (and easier) numerical tractability. On the other hand, many important results have been gleaned from pioneering field-theoretic studies of the Anderson transition [6]. Perturbative renormalization group (RG) approaches, and extensions thereof, work in the weak disorder regime, and are *a priori* inapplicable in the non-perturbative regime where the Anderson–Mott MIT would be expected to occur in the $d = 3$ case. As a result, well-defined precursors of the MIT observed even at very high temperatures, as experimentally demonstrated [7] in many systems in the form of scaling behaviour of various quantities, breakdown of Matthiessen rule and the Mooij correlation, cannot be accessed within such approaches. Thus, while the perturbative ($d + \epsilon$) [6] approaches have indeed provided a wealth of information, such approaches are insufficient at strong coupling, which is precisely the regime of interest for doped transition-metal oxide (TMO) systems, as well as systems like strongly interacting two-dimensional electron systems (in Si MOSFETs [8]) which have been found to undergo insulator–metal transitions. This is because one is always *effectively* in the strong disorder regime in strongly correlated electronic systems, where the renormalized one-electron band width is very small (caused by Hubbard band-narrowing) in the correlated metal (or Mott insulating states, where the band splitting *à la* Mott–Hubbard mechanism occurs). Consideration of such cases is out of bounds with perturbative approaches, and this requires the development of genuinely non-perturbative approaches which should be capable of:

- (i) extending the CPA to access Anderson localization effects, and
- (ii) having sufficient flexibility to incorporate effects of Mott–Hubbard physics via dynamical mean-field (DMF) or cluster-DMF approaches.

In this paper, we devise a new *cluster*-CPA technique that satisfies the above requirements. It is extremely simple to implement (it requires only the solution of N_c coupled, nonlinear equations for the Green function for a cluster with N_c sites), captures the *intracluster* correlations exactly, and is suited to further improvements (larger cluster size, incorporation of Mott–Hubbard physics). As we will show, it also reproduces the exact CPA limit [2] for the single-site cluster ($d = \infty$).

The CPA is tailor-made to describe the electron dynamics in a system with purely diagonal disorder when correlations between spatially separated disorder scatterers can be ignored, a situation which is formally exact in $d = \infty$. Extensions to include off-diagonal (hopping) disorder within the CPA framework have been proposed [3] by a variety of authors. Here, we will propose a different (related to non-local CPA) Green function technique. Using the equation-of-motion (EOM) technique, we explicitly include the *dynamical* effects of arbitrarily strong scattering from short-range correlated disorder potentials. In the process, we will make explicit contact with the problem of Anderson localization in disordered systems.

2. Model and solution

The first step is the construction of a suitable cluster model Hamiltonian incorporating *diagonal* disorder. Motivated by the results of [9], we generalize the Anderson disorder problem to finite

dimensions by mapping the full Anderson disorder model,

$$H = -t \sum_{(i,j)} (c_i^\dagger c_j + \text{h.c.}) + \sum_i v_i n_i, \quad (1)$$

to an effective model of a cluster of N_c sites embedded in an effective (dynamical) bath with a *complex* self-energy (matrix of size N_c^2). Here, we assume a binary alloy distribution for disorder, $P(v_i) = (1-x)\delta(v_i - v_A) + x\delta(v_i - v_B)$, and further, that $\langle v_i v_j \rangle - \langle v_i \rangle \langle v_j \rangle = f_{ij} \equiv C$, a constant parameter. Strictly speaking, the SRO encoded in f_{ij} is a function of x , temperature and other variables depending on the specific physical situation under consideration, and in real materials, this dependence should be explicitly taken into account. Given the choice of an embedded cluster, only consideration of non-local processes on the cluster length scale is possible (this means consideration of nearest-neighbour disorder correlations for our choice; see below). Our aim in this work is to study the electronic structure changes accompanying changes in x , $P(v_i)$ and f_{ij} for a half-filled band.

In contrast to CPA, the method described below is tailor-made to capture the dynamical effects of repeated scattering from a cluster of sites, which are correlated in a manner described by f_{ij} over the cluster length scale. To proceed, we start with the embedded cluster Hamiltonian,

$$H = -t \sum_{\alpha} (c_0^\dagger c_{\alpha} + \text{h.c.}) + v x_0 n_0 + v \sum_{\alpha} x_{\alpha} n_{\alpha} + \sum_k \epsilon_k c_k^\dagger c_k + t \sum_{k,\alpha} e^{ikR_{\alpha}} (c_{\alpha}^\dagger c_k + \text{h.c.}), \quad (2)$$

where $0, \alpha = 1, \dots, z$ denote a central site 0 coupled (via t) to z nearest neighbours on a $d = z/2$ -dimensional lattice, $x_0, x_{\alpha} = 0, 1$ for a binary disorder distribution $P(v_i)$ taking on two values: $v_i = 0$ with probability $(1-x)$ and $v_i = v$ with probability x , $\epsilon_k = \frac{1}{N} \sum_{(i,j)} t e^{ik(R_i - R_j)}$ is the band dispersion on the original lattice, and the last term describes the hybridization of site α on the boundary of the chosen cluster with an effective medium (conduction electron bath function) that has to be self-consistently determined by a suitable imbedding procedure. We describe the details in the course of the derivation below.

To proceed, we use the *exact* analogy between the problem of electronic propagation in a random, binary alloy and the so-called ‘Hubbard III’ solution for the Hubbard model [11], where one spin species ($-\sigma$ spins) is assumed to be completely static [2]. In this approximate solution of the Hubbard model, the local potential felt by a σ -spin electron switches between $v = 0$ and U depending on whether the site that it hops onto is empty or already occupied by a $-\sigma$ spin electron. In the disordered, paramagnetic phase, this maps *exactly* to the random alloy problem we consider here. Given this analogy, we choose to solve the disorder problem using an extension of the two-time Green function method used by Hubbard (it is now known that the Hubbard III solution is actually the exact solution for the one-particle Green function of this ‘simplified’ Hubbard model in $d = \infty$). This exact analogy means that x_{α} above can be exactly identified with $n_{-\sigma}$ in the Hubbard III formulation.

Defining the diagonal and off-diagonal propagators on the cluster as $G_{00}(\omega) = \langle c_0; c_0^\dagger \rangle$, $G_{k0}(\omega) = \langle c_k; c_0^\dagger \rangle$, $G_{\alpha 0}(\omega) = \langle c_{\alpha}; c_0^\dagger \rangle$, we start with the equation of motion (EOM) for $G_{00}(\omega)$:

$$\omega G_{00}(\omega) = 1 + t \sum_{\alpha} G_{\alpha 0}(\omega) + v \langle x_0 c_0; c_0^\dagger \rangle. \quad (3)$$

Notice the appearance of a ‘higher-order’ Green function (in analogy with Hubbard III) on the rhs of equation (3). It is naturally interpreted as the probability amplitude for having an electron at a site 0 with disorder potential v . Its EOM reads

$$(\omega - v) \langle x_0 c_0; c_0^\dagger \rangle = \langle x_0 \rangle + t \sum_{\alpha} \langle x_0 c_{\alpha}; c_0^\dagger \rangle. \quad (4)$$

The EOM for $G_{\alpha 0}(\omega)$ on the rhs of equation (3) reads

$$\omega G_{\alpha 0}(\omega) = v \langle x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle + t G_{00}(\omega) + t \sum_k G_{k0}(\omega), \quad (5)$$

and in a way similar to that leading to equation (4), we obtain

$$(\omega - v) \langle x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle = t \langle x_{\alpha} c_0; c_0^{\dagger} \rangle + t \sum_k \langle x_{\alpha} c_k; c_0^{\dagger} \rangle. \quad (6)$$

Continuing along with identical lines for the various ‘higher-order’ Green functions generated in equations (3)–(5) gives us

$$\omega \langle x_0 c_{\alpha}; c_0^{\dagger} \rangle = v \langle x_0 x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle + t \langle x_0 c_0; c_0^{\dagger} \rangle + t \sum_k \langle x_0 c_k; c_0^{\dagger} \rangle, \quad (7)$$

$$\omega \langle x_{\alpha} c_0; c_0^{\dagger} \rangle = \langle x_{\alpha} \rangle + v \langle x_{\alpha} x_0 c_0; c_0^{\dagger} \rangle + t \langle x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle, \quad (8)$$

$$(\omega - v) \langle x_0 x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle = t \langle x_0 x_{\alpha} c_0; c_0^{\dagger} \rangle + t \sum_k \langle x_0 x_{\alpha} c_k; c_0^{\dagger} \rangle \quad (9)$$

and

$$(\omega - v) \langle x_{\alpha} x_0 c_0; c_0^{\dagger} \rangle = \langle x_0 x_{\alpha} \rangle + t \langle x_0 x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle. \quad (10)$$

Finally,

$$(\omega - \epsilon_k) \langle A_{0\alpha} c_k; c_0^{\dagger} \rangle = t_k \langle A_{0\alpha} c_{\alpha}; c_0^{\dagger} \rangle, \quad (11)$$

where $A_{0\alpha} = 1, x_0, x_{\alpha}, x_0 x_{\alpha}$ for the various types of Green functions which couple the bath back to the cluster (see above), and $\langle x_{0\alpha} \rangle \equiv \langle x_0 x_{\alpha} \rangle$ is the non-local correlation function of the disorder potential over the cluster length scale, involving only nearest neighbours for our choice of cluster (scaling like $1/d$ in d dimensions). Here, t_k is the ‘hybridization’ which couples the boundary sites α to the bath of ‘conduction electrons’, and is physically identical to the one-electron hopping term in the original lattice model. For a single-site cluster, we recover the *exact* CPA result using the EOM for $G_{00}, G_{k0}, \langle x_0 c_0; c_0^{\dagger} \rangle$ and $\langle x_0 c_k; c_0^{\dagger} \rangle$ only. Indeed, in the single-site limit, the local Green function at the site 0 is easily seen to be

$$G_{00}(\omega) = \frac{1 - \langle x_0 \rangle}{\omega - \Delta(\omega)} + \frac{\langle x_0 \rangle}{\omega - v - \Delta(\omega)}, \quad (12)$$

which is exactly the CPA (or the Hubbard III, with $\langle x_0 \rangle = \langle n_{-\sigma} \rangle$) result when we use the fact that $\Delta(\omega) = t^2 G_{00}(\omega)$ for the Bethe lattice, leading to the cubic equation for G_{00} derived by Hubbard.

In our cluster generalization, after a long and somewhat tedious algebra, we finally find

$$G_{00}(\omega) = \frac{1 + v \langle x_0 c_0; c_0^{\dagger} \rangle + (v/t) F_2(\omega) \langle x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle}{\omega - z F_2(\omega)} \quad (13)$$

and

$$G_{\alpha 0}(\omega) = \frac{1}{\omega - \Delta(\omega)} \frac{v \omega \langle x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle + t(1 + v \langle x_0 c_0; c_0^{\dagger} \rangle)}{\omega - z F_2(\omega)}, \quad (14)$$

where

$$v \langle x_0 c_0; c_0^{\dagger} \rangle = \frac{v \langle x_0 \rangle + (v/t)^2 \langle x_0 x_{\alpha} \rangle \frac{F_1(\omega) F_2(\omega)}{\omega - v - F_1(\omega)}}{\omega - v - F_2(\omega)} \quad (15)$$

and

$$\langle x_{\alpha} c_{\alpha}; c_0^{\dagger} \rangle = t^{-1} F_1(\omega) \langle x_{\alpha} c_0; c_0^{\dagger} \rangle, \quad (16)$$

with

$$\langle x_\alpha c_0; c_0^\dagger \rangle = \frac{\langle x_\alpha \rangle - \langle x_0 x_\alpha \rangle}{\omega - F_1(\omega)} + \frac{\langle x_0 x_\alpha \rangle}{\omega - v - F_1(\omega)}. \quad (17)$$

Here, $F_1(\omega) \equiv \frac{t^2}{\omega - v - \Delta(\omega)}$ and $F_2(\omega) \equiv \frac{t^2}{\omega - \Delta(\omega)}$. Finally, the bath function, $\Delta(\omega)$ is computed from the equation [11, 12]

$$G_{00}(\omega) = \int_{-W}^{+W} \frac{\rho_0(\epsilon) d\epsilon}{G_{00}^{-1}(\omega) + \Delta(\omega) - \epsilon}, \quad (18)$$

where ρ_0 is the unperturbed (disorder-free) density of states (DOS).

It is instructive to point out here that the self-consistency condition (equation (18)) looks like the usual self-consistency condition of single-site DMFT. This is so because the coupling of the cluster to the ‘bath’ (i.e., the rest of the lattice) is bilinear in the fermions. However, we draw attention to the fact that $G_{00}(\omega)$ is the onsite Green function of the *cluster* problem, explicitly dependent on $f_{0\alpha} = \langle x_0 x_\alpha \rangle - \langle x_0 \rangle \langle x_\alpha \rangle$ via equation (13) above. This last feature is directly related to the explicit incorporation of intersite correlations of the disorder potentials, and drops out in $d = \infty$ (it scales as $1/d$). Obviously, the bath function also depends explicitly on $f_{0\alpha}$, in contrast to usual CPA, where it can only depend on $\langle x_\alpha \rangle$ by construction.

At this point, one can show that the cluster-CPA technique developed above always yields a positive-definite local DOS, defined by $\rho(\omega) = -\text{Im } G_{00}(\omega)/\pi$. To show this explicitly, we observe that $G_{00}(\omega)$ can be brought to a convenient mathematical form by simple algebraic manipulations:

$$G_{00}(\omega) = \frac{1 - \langle x_0 \rangle}{\omega - F_2(\omega)} + \frac{\langle x_0 \rangle}{\omega - v - F_2(\omega)} - \left[\frac{\langle x_\alpha \rangle - \langle x_0 x_\alpha \rangle}{\omega - F_2(\omega)} + \frac{\langle x_0 x_\alpha \rangle}{\omega - v - F_2(\omega)} \right] + \frac{\langle x_\alpha \rangle - \langle x_0 x_\alpha \rangle}{\omega - F_1(\omega)} + \frac{\langle x_0 x_\alpha \rangle}{\omega - v - F_1(\omega)}. \quad (19)$$

The first step in the derivation is to notice that each of the numerators is always positive-definite by definition. Clearly, to show that $\rho(\omega)$ is always positive-definite, we have now only to show that $\text{Im } \Delta(\omega) \leq 0$. From the EOM technique used above, $\Delta(\omega) = t^2 G_{00}(\omega)$ for the Bethe lattice. A straightforward calculation shows that $\text{Im } \Delta(\omega) \leq 0$ for any choice of the unperturbed DOS, $\rho_0(\epsilon) \geq 0$. Substitution in $G_{00}(\omega)$ above immediately shows that the disorder-averaged DOS is always positive-definite (clearly, self-consistency does not modify this conclusion).

A few clarifications concerning the physical meaning of the set of equations are in order at this point. It is also easy to check that the system of equations are exact both in the band and the atomic limit, and the CPA result is readily recovered for the single-site cluster. First, we notice that the cluster Green functions are explicit functions of the higher-order (in $1/d$) SRO correlator, $\langle x_0 x_\alpha \rangle$. To interpret the meaning of the bath function, $\Delta(\omega)$ in our approach, we begin by observing that one can view *any* self-consistent cluster approximation as being a valid description in a regime with SRO on the cluster length scale (analogous to the single-site approximation being formally exact at mean-field level). An exact solution of the problem implies consideration of an infinite cluster, and, of course, is an insoluble problem. Our choice for $\Delta(\omega)$ above is then linked to the mathematical consideration of short-range correlations over the cluster length scale only, or, equivalently, to the consideration of dynamical effects of repeated scattering by a cluster consisting of a central site plus its z nearest neighbours only. The effects of non-local SRO appears explicitly in the bath function $\Delta(\omega)$ (i.e., in equation (18)) via $G_{00}(\omega)$ as defined in equation (13) with its explicit dependence on $f_{0\alpha}$. It follows that the approach describes the carrier dynamics in a situation where the carrier mean-free path is of

the order of the size of the chosen cluster ($l \simeq a$, the lattice constant for our cluster) in a fully self-consistent way (see below), one step beyond the CPA where $l = 0$.

It is interesting to notice that $G_{00}(\omega)$, $G_{\alpha 0}(\omega)$ can be (formally) analytically expressed in terms of the corresponding diagonal and off-diagonal cluster self-energies $\Sigma_{00}(\omega)$, $\Sigma_{\alpha 0}(\omega)$ for $d = 1, 2, \dots, \infty$, as well as on certain special lattices. The above set of equations then constitutes a closed set of simultaneous nonlinear equations for the two self-energies, and they are solved self-consistently to yield the renormalized (by disorder) DOS at the central site, $\rho(\omega) = -\frac{1}{\pi} \text{Im} G_{00}(\omega)$.

The alloy correlation function (describing SRO) is given by $\langle x_0 x_\alpha \rangle = \langle x_0 \rangle \langle x_\alpha \rangle + f_{0\alpha}$ in the general case, with $f_{0\alpha}$ encoding complete information about order–disorder instabilities in the alloy. It is important to notice that the *dynamical* effect of strong scattering by these short-range correlations ($f_{0\alpha}$) on the electronic self-energy is explicitly included within our formulation above. In particular, the electron can undergo repeated scattering on the atomic sites within the chosen cluster, and, depending upon the degree and character of SRO (see below), can be localized due to interference effects coming from repeated scattering from spatially separated centres; i.e., via Anderson localization. To address the issue of Anderson localization in our non-local CPA (NLCPA) scheme, we follow Economou *et al* [10] and use the localization function defined by

$$L(\omega) = Kt \left| G_{00}(\omega) - \frac{G_{0\alpha}(\omega)G_{\alpha 0}(\omega)}{G_{00}(\omega)} \right|, \quad (20)$$

where electronic eigenstates with energy ω satisfying

- $L(\omega) > 1$ define *extended* states,
- $L(\omega) < 1$ define Anderson localized states, and,
- $L(\omega) = 1$ defines the mobility edge.

Here, K is the connectivity of the lattice. The formalism developed above thus allows one to determine the boundary between localized and extended states and its dependence on lattice structure, type of SRO, and band-filling. We are presently unable to compute the localization length and its critical behaviour as the Anderson transition is approached. This is mainly related to the prohibitive numerical cost involved in treating larger clusters. Let us, however, point out that Economou *et al* [10] have even used the single-site CPA to evaluate the localization criterion. More recently, Dobrosavljević *et al* [13] have used related ideas, again using the CPA propagator, to study Anderson localization. Our approach extends these calculations by explicitly incorporating intersite alloy correlations in the cluster Green functions, as emphasized above (cf equations (3)–(18)). Of course, events corresponding to ‘rare’ potential fluctuations cannot be easily incorporated into a cluster theory such as ours. Hence, such cluster approximations *cannot* yield the DOS tails, a feature they share with single-site DMF theory.

3. Numerical results and discussion

In this section, we describe the results obtained from the numerical solution of the self-consistent set of coupled nonlinear equations derived in the previous section. Since we are interested in the generic effects of atomic SRO on the carrier dynamics, we choose the semicircular unperturbed DOS $\rho_0(E) = \frac{2}{\pi W^2} \sqrt{W^2 - E^2}$ as an approximation to the actual DOS for a three-dimensional cubic lattice [11]. This leads to a considerable simplification in the numerics without affecting the generic features qualitatively. We work with $W = 1.424$ eV and study the fully renormalized DOS, $\rho(\omega)$ and $L(\omega)$ as functions of the alloy composition

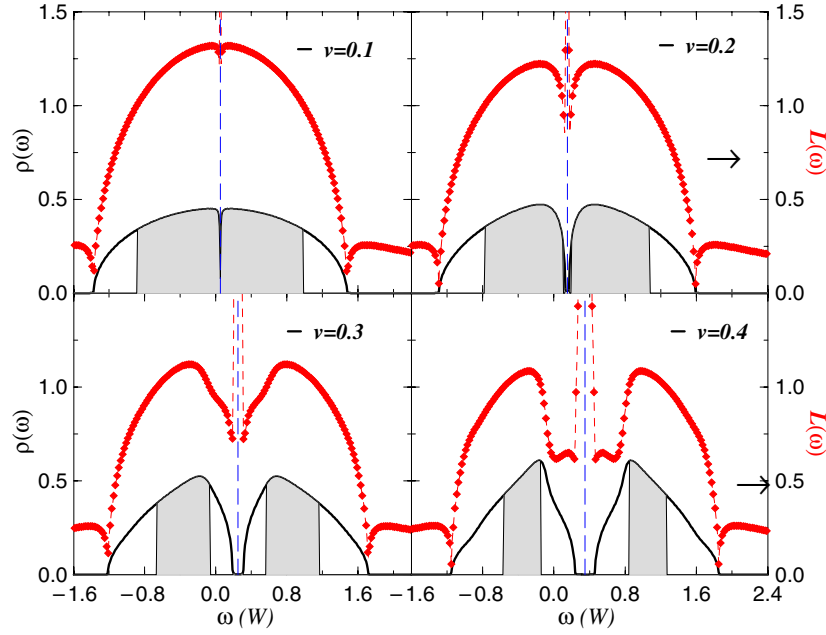


Figure 1. Cluster-CPA DOS the binary-alloy distribution in the extreme SRO limit on a Bethe lattice for $\langle x_0 \rangle = 0.5$, $\langle x_{0\alpha} \rangle = 0.0$ and various values of the local disorder potential, $v = 0.1, 0.2, 0.3, 0.4$. Shaded regions define extended states, and unshaded regions define Anderson localized states.

$y = (\langle x_0 \rangle / (1 - \langle x_0 \rangle))$, the atomic SRO parameter $f_{0\alpha}$ and the disorder strength v for a half-filled band.

Before describing our results, it is instructive to consider the correctness of the formalism in special limiting cases. As is obvious from equations (13)–(19), the correct band and atomic limits are reproduced, as is the CPA for a single-site cluster. Further, $\langle x_0 x_\alpha \rangle = \langle x_0 \rangle \langle x_\alpha \rangle + f_{0\alpha} = x^2 + f_{0\alpha}$ with $f_{0\alpha} = 0$ for a completely random alloy. In the general case, the small- x limit, the random scatterers are far apart from each other, so that $f_{0\alpha} = 0$ in our cluster problem for scatterers separated by a distance $R > \xi$, the largest cluster size under consideration. Using equation (19), we get

$$G_{00}(\omega) = (1 - x) \left[\frac{1 - x}{\omega - F_2(\omega)} + \frac{x}{\omega - v - F_2(\omega)} \right] + x \left[\frac{1 - x}{\omega - F_1(\omega)} + \frac{x}{\omega - v - F_1(\omega)} \right], \quad (21)$$

showing that our pair-cluster approximation indeed gives the correct behaviour for the Green function ($\simeq x^2$) in the small- x limit. This fulfils one of the acceptable criteria for an acceptable ‘p-centre’ approximation. Finally, we have checked that our renormalized cluster DOS intersects the CPA DOS eight times, implying that our cluster extension exactly reproduces the first *eight* moments of the DOS (cf CPA, which reproduces the first seven moments exactly).

We begin with the symmetric case with $y = 1$, and extreme random disorder, i.e., $f_{0\alpha} = 0$ or $\langle x_{0\alpha} \rangle = \langle x_0 \rangle \langle x_\alpha \rangle$. In $d = \infty$, this corresponds to the CPA, with the metal–insulator transition occurring *continuously* at $v \geq W$. Inclusion of SRO drastically changes the picture. The M–I transition now occurs much earlier. In fact, the band-split regime occurs for $v/W \geq 1/4$. However, states near and at the band centre become Anderson localized *before* the band splits

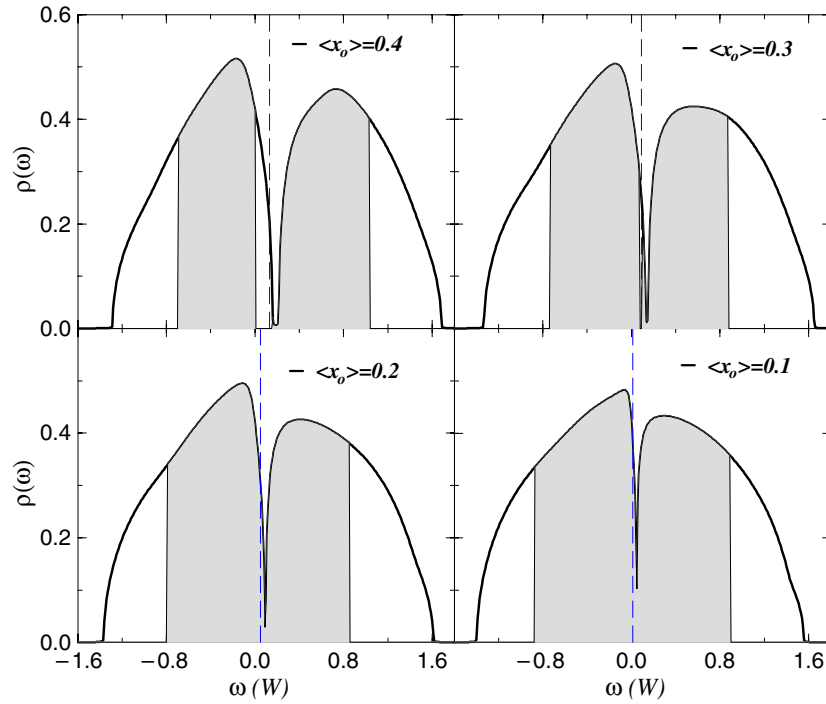


Figure 2. Cluster-CPA DOS on a Bethe lattice for $\langle x_{0\alpha} \rangle = 0.0$, $v = 0.5$ and different alloy concentrations, $\langle x_0 \rangle = 0.4, 0.3, 0.2, 0.1$.

(figure 1) and the metal (incoherent)–Anderson insulator transition is continuous. For $v < v_c$, the incoherent metal has a very similar character (breakdown of the quasiparticle) to that found in $d = \infty$ (CPA). It is also clear that the configuration-averaged single particle DOS shows no anomalies across the Anderson localization transition, in agreement with well-known [13] arguments.

In figure 2, we show the effect of changing the alloy composition on the critical value of v needed to split the band. For the case $y = 2/3$ (i.e., $\langle x_0 \rangle = 0.4$), a larger $v_c = 0.5$ is required to localize states at E_F , and it increases to $v_c = 0.85$ for $y = 3/7$ ($x = 0.3$). This Anderson insulating state (notice that the Fermi level, denoted by the vertical lines in our plots, lies in the region of localized states) is explicitly related to our inclusion of the effect of carrier scattering on short-range intersite atomic correlations ($f_{0\alpha} = C$) and is never observed in the CPA solution ($d = \infty$), which always predicts an incoherent metal for a (half-filled band) particle–hole asymmetric disorder distribution. A continuous transition from an Anderson localized insulator to an incoherent metal is clearly seen upon decreasing y for a fixed disorder strength.

Next, we focus on the effect of varying the SRO parameter on the electronic structure. In figure 3, we show the DOS for $v = 0.5$ for different values of $\langle x_{0\alpha} \rangle = 0.1, 0.2, 0.3, 0.4$. Clearly, introducing partial order (actually, this corresponds to *increasing* $f_{0\alpha}$) results in increased tendency to itinerance, moving E_F out of the region of localized states. The AL insulator to incoherent metal transition is clearly observed with increasing $f_{0\alpha}$, and is a concrete illustration of an insulator–metal transition driven by the degree of atomic SRO (partial order) in a system. Clearly, increasing partial order (notice that increasing $f_{0\alpha}$ corresponds to increasing the probability of having the *same* potential on the cluster sites) reduces the localizing effect

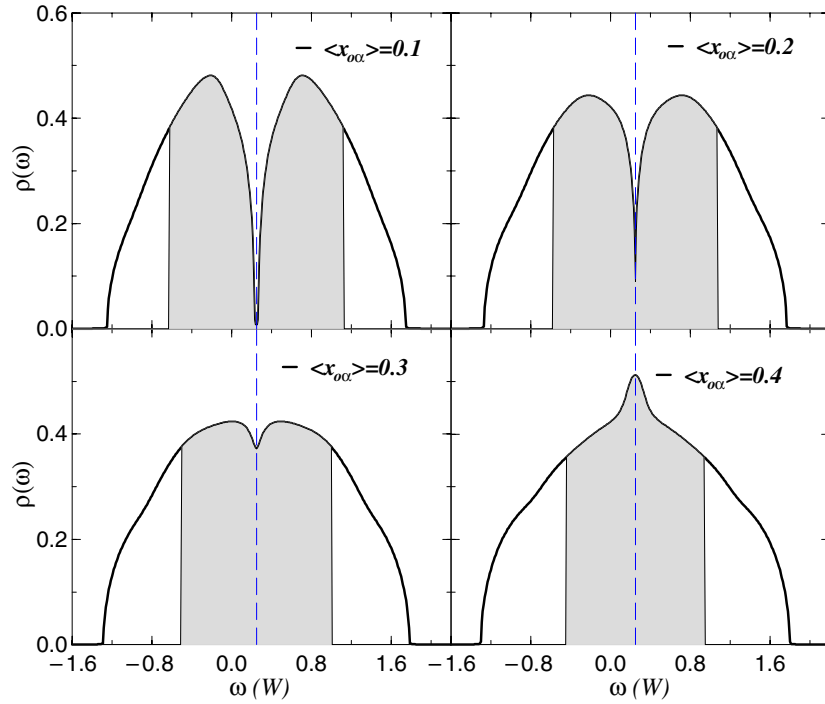


Figure 3. Effect of partial SRO on the cluster-CPA DOS for a Bethe lattice with $\langle x_0 \rangle = 0.5$, $v = 0.5$ and $\langle x_{0\alpha} \rangle = 0.1, 0.2, 0.3, 0.4$.

of strong (repeated) intracluster disorder scattering, driving the I–M transition via increased itinerance. The situation is analogous to the case where the pure Anderson disorder model is supplemented by additional short-range correlations in the hopping [14], where increasing the off-diagonal randomness drives an insulator–metal transition for a fixed diagonal disorder strength.

Qualitatively similar behaviour is seen for an asymmetric alloy distribution. In figure 4, we show the DOS for $v = 0.5$ and $y = 3/7$ (i.e., $\langle x_0 \rangle = 0.3$). Interestingly, the spectrum shows additional features, but the AL insulator–metal transition with increasing $f_{0\alpha}$ follows the trend for the symmetric ($y = 1$) case.

Increasing the ratio v/W reveals rich structures in the DOS. In figure 5, we show the one-electron DOS for $v = 1.5$ with $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$. Next, we turn our attention to figure 6, which shows the evolution of the DOS for the asymmetric alloy distribution with $\langle x_0 \rangle = 0.3$ for the same parameters. In this case, we are already in the split-band regime. Very rich structure is seen in the results. For comparison, we know that the corresponding DOS obtained for these cases within the CPA ($d = \infty$, not shown) shows a split-band structure with only upper and lower ‘Hubbard’ bands. Obviously, the CPA is incapable of resolving the fine structure in the DOS originating from repeated scattering between spatially separated scattering centres. The rich structures seen in the cluster generalization correspond partially to these effects, and can be traced back to the spectrum of eigenstates of the isolated cluster. In fact, the multiple subbands can easily be shown to be centred around eigenenergies of the isolated cluster for the case of the symmetric alloy distribution with $f_{0\alpha} = 0$. However (figures 5 and 6), in the general case with $f_{0\alpha} \neq 0$, one sees eight or nine distinct subband structures. We interpret the additional structures as arising from atomic SRO (non-zero $f_{0\alpha}$);

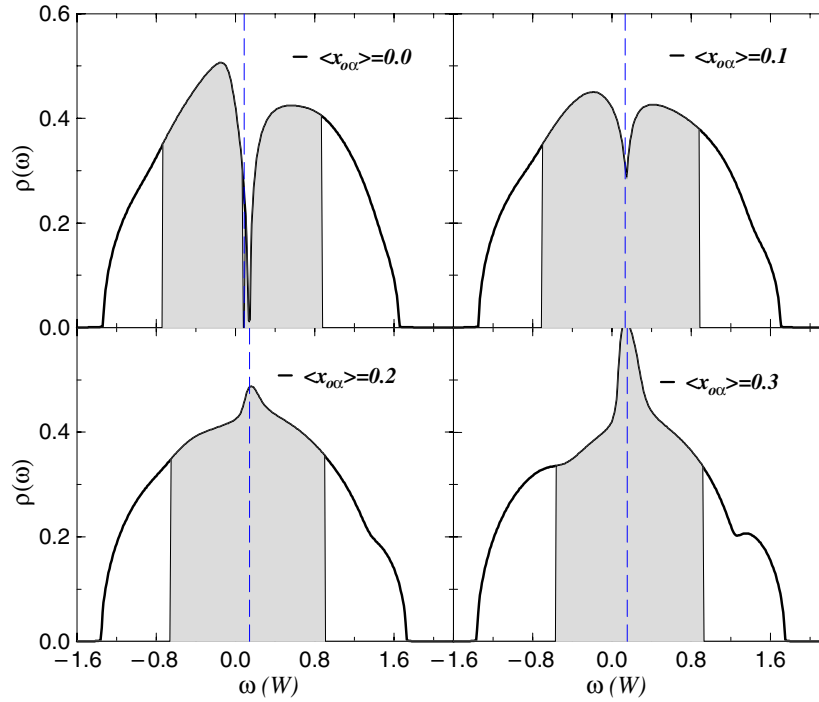


Figure 4. Effect of partial SRO on the cluster-CPA DOS for a Bethe lattice with $\langle x_0 \rangle = 0.3$, $v = 0.5$ and $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$.

in particular from ‘shake-up’ effects originating from strong resonant scattering of carriers (from the atomic SRO) from cluster sites. For comparison, we remark that coupling the two-site cluster to the ‘bath’ (rest of the lattice) via second-order processes in the hopping (corresponding to the ‘Hubbard I’ approximation for the cluster) is incapable of accessing SRO effects in a consistent way. In particular, in addition to violating the Hubbard sum rules [15], it cannot yield ‘shake-up’ features in the DOS, always yielding *only* six bands centred around the eigenvalues of the two-site cluster, and broadened by an amount $O(t)$. This discussion shows the importance of treating the effects of *both* itinerance (via $\Delta(\omega)$) and the (incoherent) resonant scattering on the same footing, and reveals the weaknesses inherent in uncontrolled approximations.

Additional interesting features observed from the calculations deserve comments. We clearly observe that the localization function $L(\omega)$ shows non-analytic behaviour near each subband edge, but no non-analyticities across the mobility edge. More detailed characterization of the Anderson insulator–metal transition requires a detailed study of the two-particle responses [16](density correlations, optical conductivity), and is left for future work.

Given the close analogy between the problem of electron propagation in a random alloy and the Hubbard III solution in the paramagnetic disordered state, we expect that our formulation employing the equations-of-motion technique for two-time Green functions can also be rewritten in the t -matrix formulation, along the same lines which allows the Hubbard III solution to be rewritten in alloy language, supplemented with the requirement of zero scattering ‘on the average’ in a self-consistently determined effective medium. The cluster case requires one to keep second-order terms like $\mathbf{G}_0 \mathbf{t} \mathbf{G}_0 \mathbf{t} \mathbf{G}_0$ (here, \mathbf{G}_0 and \mathbf{t} are $N_c \times N_c$ matrices for a cluster having N_c sites) in the \mathbf{t} matrix expansion linking a given site to itself ($\text{diag}[\mathbf{t}]$) as well as to its

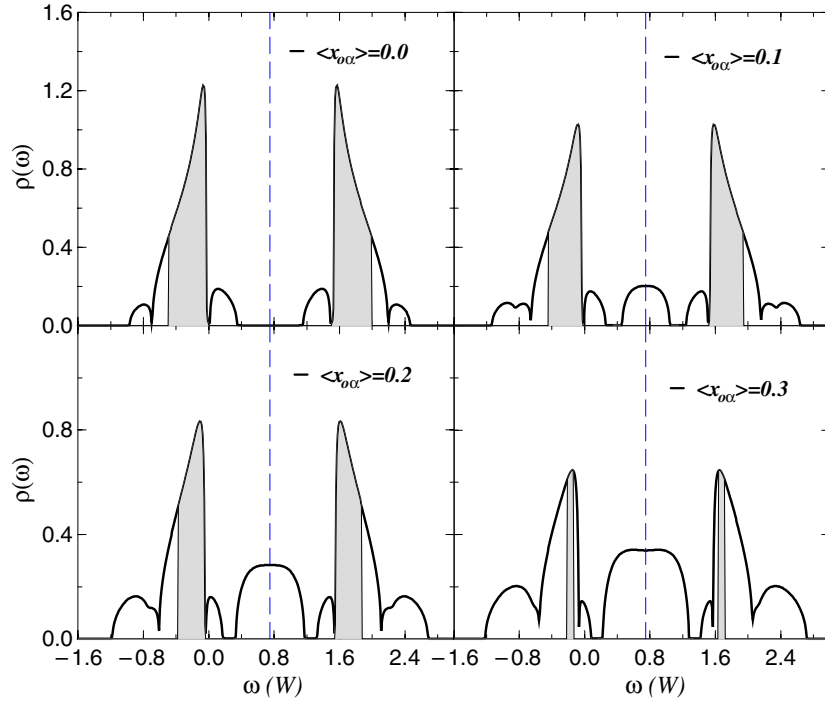


Figure 5. Cluster-CPA DOS for $\langle x_0 \rangle = 0.5$, $v = 1.5$ and $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$.

neighbours (off-diag[\mathbf{t}]), and leads one to having to solve for the matrix Green function under the simultaneous requirement $\langle t_{00} \rangle = 0 = \langle t_{0\alpha} \rangle$ ($\langle \cdot \cdot \cdot \rangle$ is the disorder average, as in CPA). While these equations have been employed in earlier works [3, 19] (indeed, a short discussion concerning this general form already appears in the original paper of Velický *et al* [2]), we are unaware of systematic incorporation of effects coming from non-zero $f_{0\alpha}$ in these earlier works.

A more rigorous test of the quality of our cluster approximation would be to apply it to the extreme case of the one-dimensional Anderson disorder problem, for which numerically exact histogram results are available. While our cluster problem does give results which are closer to the histogram results with regard to those obtained from the CPA (which, as is known, completely misses the fine structure in the DOS arising from non-local disorder fluctuations), we have found on closer inspection that incorporation of longer-range alloy correlations is necessary to obtain meaningful quantitative agreement. While this issue is being studied, and will be addressed in the future, we wish to point out that a cluster-based scheme like ours is designed for, and should be a good approximation in, spatial dimension $d > 2$ (recall [6] that for $d \leq 2$, all states are Anderson localized for any value of disorder, though the localization is weak for small disorder; this is extremely hard, if not impossible, to access with a self-consistent cluster theory). We draw attention to the fact that Rowlands *et al* [18] have studied exactly this problem keeping four sites on a chain coupled to an appropriate bath using the KKR-NLCPA (DCA), obtaining satisfactory agreement with the exact results. Our results do show some resemblance to theirs; however, more work is required to elucidate this point in more detail. In contrast to their work, we have considered the issue of Anderson localization and partial order-driven insulator–metal transitions for $d > 2$. Further, our treatment of partial SRO is very different from theirs. It is worth pointing out that our results, along with the

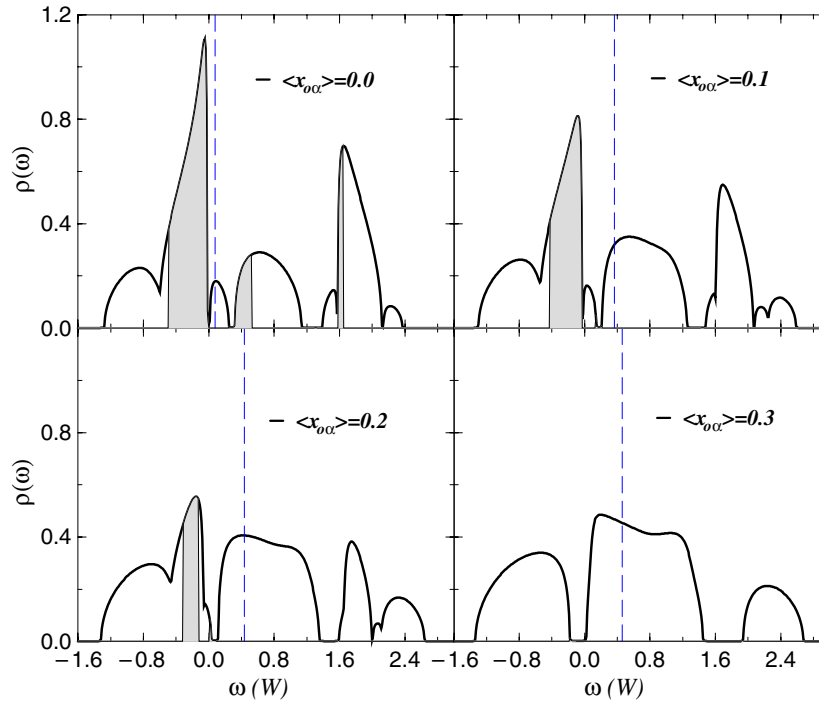


Figure 6. Cluster-CPA DOS for $\langle x_0 \rangle = 0.3, v = 1.5$ and $\langle x_{0\alpha} \rangle = 0.0, 0.1, 0.2, 0.3$.

NLCPA ones, are quite different from those obtained by Jarrell *et al* [5]. However, we are presently unable to quantify the reasons behind these differences.

Finally, our approach shares some formal similarities with the one developed by Miwa *et al* [17]. There are some notable differences, however, between our approach and theirs. First, their approach is based on the t -matrix formulation and a locator expansion for the local Green function, while ours is based on the equation-of-motion technique for two-time Green functions, *à la* Hubbard III. While they expect to capture two more moments beyond CPA, this is not shown explicitly there. Our technique captures the first eight moments of the spectral function, as described above. Second, their approach, to our best knowledge, has not been explicitly extended to treat the effect of non-zero $f_{0\alpha}$ on the local DOS, and in particular to study the insulator–metal transition driven by increasing partial order, in contrast to our technique. Along with the other non-local CPA schemes mentioned above (except that of Jarrell *et al* [5]), the possibility of Anderson localization due to finite $f_{0\alpha}$ has not been considered. The advantage of our formulation is that it allows a study of such effects to be carried out. Further, we have shown that our DOS is always positive definite, and so we believe that our cluster extension is analytic in the complex energy plane. An explicit derivation of analyticity of our cluster-CPA technique will be presented separately.

We emphasize that the approach developed here has a wide applicability to various strong coupling cases in three dimensions where the effect of atomic (chemical), magnetic, Jahn–Teller, etc, SRO on the character of carrier dynamics is an important issue. In particular, it should be applicable to the problem of electronic structure of disordered transition-metal alloys [19, 17], and to more recent cases such as hole-doped manganites [20], where a plethora of experimental work clearly demonstrates the importance of such effects in a correlated environment. Applications to such systems are in progress and will be reported elsewhere.

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