Systems with static and dynamic disorder: generalised coherent potential approximation

Systems with static and dynamic disorder: generalised coherent potential approximation

Abhijit Mookerjee

Department of Physics, Indian Institute of Technology, Kanpur 208016, India

Abstract. Using the ideas of the augmented space formalism introduced some time ago by this author, a generalisation of the coherent potential approximation and its cluster extensions is developed for systems that have both inherent static disorder as well as potentials that fluctuate randomly with time. The formalism reduces to standard results in the adiabatic limit.

1. Introduction

The standard method of dealing with electronic systems in contact with a thermal (phonon) bath is to assume that the timescales associated with the electronic motion (τ_e, where τ_e is the timescale associated with the system of electrons coupled to the random bath) and the bath (τ_b) are very different. If $\tau_e \ll \tau_b$, then we may decouple the electronic and phonon degrees of freedom. This is the adiabatic approximation. We assume that for $t < \tau_e$ the phonon degrees of freedom are frozen and the electrons essentially move in a potential that deviates from their perfect values in the absence of the bath (Born–Oppenheimer). However, there are situations where this breaks down and $\tau_e \simeq \tau_b$. Certain two-level systems near $T = 0$ and near localised, sluggish conduction electrons in the so-called Mooij alloys are some examples of this.

The aim of this paper is to develop a formalism that would deal, in a unified manner, with situations where there is inherent static (quenched) disorder (as in random alloys, distorted lattices and networks) as well as dynamic disorder, because of coupling to a noise bath. In addition, the adiabatic approximation may not hold. Our approach will be based on the augmented space technique, which was proposed for static disorder problems by this author (Mookerjee 1973). Recently, Paquet and Leroux-Hugon (1984) have introduced a dynamic coherent potential approximation (CPA) based on the augmented space technique referred to above and have applied it to interesting examples of two-level systems.

The aim of this work is to improve upon these earlier ideas in the following specific way: in the earlier treatments the dynamic disorder was treated within perturbation theories, while the static disorder was treated within more sophisticated mean-field approaches like the CPA or its cluster versions. The assumption made, though not explicitly stated, was that the effects of static and dynamic disorder are uncorrelated. This latter assumption is shown to be invalid in specific examples. We shall treat both

the static and dynamic disorders on the same footing on the augmented space, combining the work of Paquet and Leroux-Hugon (1984) with our earlier approach for static disorder.

2. The augmented space formalism

2.1. Static disorder

The augmented space formalism was introduced by this author (Mookerjee 1973) to deal with the problem of averaging over static disorder configurations. The formalism puts configuration averaging on the same footing as quantum-mechanical averaging, by augmenting the Hilbert space spanned by the wavefunctions by a *disorder* or *configuration* space spanned by the different *configuration states*. The algebra of the method has been discussed in detail earlier (Gray and Kaplan 1976, Kaplan and Gray 1982). Here we shall pick up a typical example to bring out the connection with our subsequent treatment of dynamic disorder.

Suppose that the Hamiltonian describing a system is characterised by a set of independent random variables $\{x_i\}$. The probability density of $\{x_i\}$ is assumed to have finite moments to *all* orders so that we may write

$$p(x_i) = (-1/\pi) \, \text{Im} \langle \gamma_0^i | [(x_i + i0)I - M^{(i)}]^{-1} | \gamma_0^i \rangle \tag{1}$$

where $M^{(i)}$ is an operator on a space $\Phi^{(i)}$ of rank N, spanned by the N possible configurations of x_i. Even if x_i has continuous values, a countable basis $|\gamma_m^i\rangle$ may still be chosen, but the rank of $\Phi^{(i)}$ now becomes infinite.

A suitable choice of the basis is one that makes $M^{(i)}$ tridiagonal. This tridiagonal representation may be immediately obtained by looking at the continued-fraction expansion for $p(x_i)$:

$$p(x_i) = -\frac{1}{\pi} \, \text{Im} \, \cfrac{1}{x_i - a_1 - \cfrac{b_1^2}{x_i - a_2 - \cfrac{b_2^2}{\cdots}}}. \tag{2}$$

Since $p(x_i) \geq 0$ and has finite moments to *all orders*, it always has a convergent continued-fraction expansion with real coefficients $\{a_n, b_n\}$. The representation of $M^{(i)}$ has a_n down the diagonal and b_n down the off-diagonal positions.

The formalism now states that the configuration average over any function of $H(\{x_i\})$, $\mathcal{F}$, may be written

$$\int P(\{x_i\}) \mathcal{F}[H(\{x_i\})] \, \mathrm{d}\{x_i\} = \langle f | \tilde{\mathcal{F}}[\tilde{H}] | f \rangle \tag{3}$$

where $\tilde{\mathcal{F}}$ is the same functional operator of $\{M^{(i)}\}$ as $\mathcal{F}$ was a function of $\{x_i\}$ and $|f\rangle = \Pi^\otimes |\gamma_0^i\rangle$ is the configuration *ground state*. The configuration averaging has been reduced to the problem of the ground-state matrix element in the augmented space $\Psi = \mathcal{H} \times \Phi$ where $H \in \mathcal{H}$ and $\Phi = \Pi^\otimes \varphi^{(i)}$, an idea familiar in quantum-mechanical *averaging*.
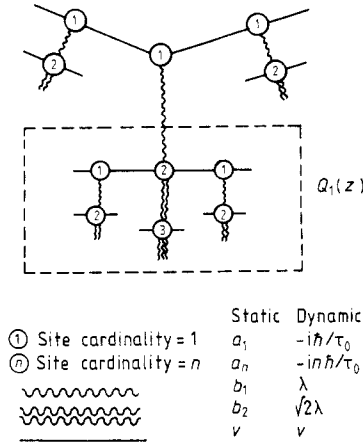
Figure 1. Part of the delinked graph for the single-site CPA on a disorder problem both static and dynamic.

Since the basis in $\Phi^{(i)}$ is countable, we shall define the *cardinality* of $|\gamma_n^i\rangle$ to be the integer n

$$\text{card}|\gamma_n^i\rangle = n \qquad \text{card}\{|\gamma_n^i \otimes \gamma_m^i\rangle\} = n + m. \tag{4}$$

We shall introduce the notation $|f_{n,q}^i\rangle$ to denote any member of the set $|\gamma_{n_1}^1 \otimes \gamma_{n_2}^2 \otimes \ldots \otimes \gamma_n^i \otimes \ldots\rangle$ with card $|f_{n,q}^i\rangle = q$.

Suppose we have a Hamiltonian $H \in \mathcal{H}$ of the form

$$H = \sum \varepsilon_i P_i + \sum \sum V_{ij} T_{ij} \tag{5}$$

where the basis in $\mathcal{H}$ is a suitably chosen orthogonal, site-labelled set $|r_i\rangle$ which spans $\mathcal{H}$. The *augmented space theorem* then states that, if the set of diagonal terms $\{\varepsilon_i\}$ is identified with the random set $\{x_i\}$, then

$$\tilde{H} = \sum_i \tilde{M}^{(i)} \otimes P_i + \sum_i \sum_j V_{ij} \tilde{I} \otimes T_{ij} \tag{6}$$

and

$$\langle G(z)\rangle_{\text{av}} = \langle f|(z\tilde{I} - \tilde{H})^{-1}|f\rangle$$

with

$$\tilde{M}^{(i)} = I \otimes I \otimes \ldots \otimes M^{(i)} \otimes \ldots \otimes I.$$

To obtain the self-energy in the CPA, for example, we shall follow the graphical approach of Haydock (1972, 1980). The method is equivalent to and an alternative of the *t*-matrix approach. Although the latter is the more familiar, the former has the advantage of making the structure of the approximating terms more transparent. It was shown earlier (Bishop and Mookerjee 1974) that calculating the Green function on the graph for $\tilde{H}$ in the augmented space, which is modified in such a way that all closed paths that do not lie entirely in a subspace spanned by a basis of the same cardinality are delinked, leads exactly to the single-site CPA. Figure 1 shows a part of the delinked graph for $\tilde{H}$. The self-energy arises because of the decorations of the original lattice in $\mathcal{H}$

by augmented space *decorations*. It is clear that the delinking leads to a self-energy completely diagonal in the space $\mathcal{H}$. Let us examine this graph:

$$\Sigma(z) = a_1 + b_1^2 Q_1(z).$$

$Q_1(z)$ is the diagonal element of the Green function of a Hamiltonian whose graph is identical to that for $\tilde{H}$ *except* that the decoration at the site r_i is $\Sigma_2(z) + a_2$ instead of $\Sigma(z)$. Thus

$$Q_1(z) = \langle r_i | [zI - H_0 - \Sigma + P_i(\Sigma - \Sigma_2 - a_2)P_i]^{-1} | r_i \rangle$$

$$= \frac{F(z)}{1 + (\Sigma - a_2)F(z) - \Sigma_2 F(z)}.$$

Here H_0 is the non-random part of the original Hamiltonian, $F(z) = g_{ii}(z - \Sigma)$ where $g = (zI - H_0)^{-1}$.

Again, if we examine the next stage of the graph:

$$\Sigma_2(z) = b_2^2 Q_2(z)$$

where again $Q_2(z)$ is the diagonal part of the Green function of a Hamiltonian whose graph is identical to that for H except that the decoration at r_i is $\Sigma_3(z) + a_3$. The recursive structure is now quite apparent and we may immediately write down the expression

$$\Sigma(z) = a_1 + \cfrac{b_1^2}{[1/F(z)] - (\Sigma + a_2) - \cfrac{b_2^2}{[1/F(z)] - (\Sigma + a_3) - \cfrac{b_3^2}{\cdots}}}. \tag{7}$$

This expression is the same as that of Sumi (1977) and the static limit structure of the self-energy of Paquet and Leroux-Hugon (1984). Contrary to the latter's comment, the graphical technique is not cumbersome; on the contrary, it brings out the recursive structure of the self-energies, which is the basis of the continued-fraction form. For the case when $p(\varepsilon_i)$ is a semi-elliptic distribution with W, $a_n = 0$ and $b_n = W/2$ for *all* n, and we immediately obtain from (7) the well known result $\Sigma = (W^2/4)F(z)$.

2.2. Dynamic disorder

Let us now discuss the case of an electric system described by a non-random Hamiltonian H_0 in contact with a stochastic bath described by a potential $\{\lambda x_i(t)\}$, where $x_i(t)$ takes a continuous set of values (say, the position of the potential centre):

$$H = H_0 + \sum \lambda x_i(t)P_i \qquad H \in \mathcal{H}.$$

We shall limit ourselves to Markovian noise. The Markov processes are the simplest possible processes that account for correlation time for the noise. The evolution probability $|p^{(i)}\rangle$ of a *stationary* Markov process is governed by the Chapman–Kolmogorov equation

$$(\partial/\partial t - \mathbb{F}^{(i)})|p^{(i)}\rangle = 0. \tag{8}$$

The Fokker–Planck operator $\mathbb{F}^{(i)}$ has a representation

$$\mathbb{F}^{(i)} = -\frac{\partial}{\partial x} v(x) - \frac{1}{2}\frac{\partial^2}{\partial x^2} d(x)$$

in the basis of continuous states $\{x\}$ of x_i, where $v(x)$ is the local velocity and $d(x)$ the

local diffusion coefficient. For the *Ehrenfest* process $v(x) = -x/\tau_0$ and $d(x) = 2/\tau_0$, where τ_0 has the interpretation of being the lifetime in the *ground state*. The stationary solution of (8) in this representation is

$$p_*^{(i)}(x) = (2\pi)^{-1/2} \exp(-x^2/2).$$

The eigenvalues of $\mathbb{F}^{(i)}$ are $-n/\tau_0$ and the corresponding eigenfunctions $|\gamma_n^i\rangle$ have a representation

$$\gamma_n^i(x) = (2^n n |\pi)^{-1/2} H_n(x/2) \exp(-x^2/2).$$

Note that $p_*^{(i)}(x) = \gamma_0^i(x)$ and any *inner product* in this representation is

$$\langle \gamma_n^{(i)} | \mathbb{A} | \gamma_m^{(i)} \rangle = \int \int dx \, dy \, \gamma_n^i(x)^* (1/p_*^{(i)}) \mathbb{A}(x, y) \gamma_m^i(x).$$

The configuration space for (x_i) is then $\Phi = \Pi^\otimes \varphi^{(i)}$ spanned by $|\gamma_{n_1}^{(1)} \otimes \gamma_{n_2}^{(2)} \otimes \ldots \gamma_{n_i}^{(i)} \otimes \ldots\rangle$.

Of interest is the evolution operator averaged over the different *histories* of the process. This may be expressed in terms of a conditional evolution operator $U(t)$ whose representation in the above basis is $U(\{x\}, \{y\}, t)$ and gives the evolution of a *history* with a starting state $\{y\}$ at $t = 0$ and a final state $\{x\}$ at t

$$\langle U(t) \rangle = \int \int d\{x\} \, d\{y\} \prod p_*(x_i)[1/p_*(x_i)] U(\{x\}, \{y\}, t) p_*(y_i)$$

that is

$$\langle U(t) \rangle = \langle f | \tilde{U} | f \rangle$$

where

$$|f\rangle = \Pi^\otimes |\gamma_0^i\rangle. \tag{9}$$

The similarity with the static disorder case is now evident. We may go further and deduce the differential equation for $\tilde{U}(t)$. Two types of evolutions are involved in this system: quantum-mechanical evolution described by the Schrödinger equation and its Hamiltonian and a Markovian evolution of the stochastic part described by the Chapman–Kolmogorov equation and the Fokker–Planck operator:

$$\tilde{U}(t + \delta t) = \tilde{U}(t) + (1/i\hbar) H \tilde{U}(t) \delta t + \sum \mathbb{F}^{(i)} \tilde{U}(t) \delta t$$

that is,

$$i\hbar \frac{\partial}{\partial t} \tilde{U} = \left(H + \sum i\hbar \mathbb{F}^{(i)} \right) \tilde{U} = \tilde{H} \tilde{U}. \tag{10}$$

Here $\tilde{H}$ is an operator in the augmented space $\mathcal{H} \otimes \Phi$. The averaged Green operator is the Laplace transform of the evolution operator

$$\langle G(z) \rangle = \langle f | (z\tilde{I} - \tilde{H})^{-1} | f \rangle. \tag{11a}$$

We may express $\tilde{H}$ in the eigenbasis of the Fokker–Planck operators. If $\{x_i(t)\}$ are taken as the positions, then using

$$\int dx \, \gamma_m^i(x^*)[1/p^*(x)] x \gamma_n^i(x) = n\delta_{m,n+1} + (n + 1)\delta_{m,n-1}$$

$$\tilde{H} = H_0 \otimes I + \sum (\lambda \tilde{M}^{(i)} \otimes P_i + i\hbar \mathbb{F}^{(i)}) \tag{11b}$$

with

$$M^{(i)} = I \otimes I \otimes \ldots M^{(i)} \otimes \ldots \qquad \mathbb{F}^{(i)} = I \otimes I \otimes \ldots \mathbb{F}^{(i)} \ldots.$$

The representation of $M^{(i)}$ is a tridiagonal matrix with $a_n = 0$ and $b_n = n$, while $\mathbb{F}^{(i)}$ are

diagonal with eigenvalues $-n/\tau_0$ down the diagonal positions. The analogy with the static case is now complete. The following comments may be made.

(i) The probability distribution $p(x)$ which corresponds to the operator $M^{(i)}$ via a relation like (1) is the Gaussian $(2\pi)^{-1}\exp(-x^2/2)$. This follows directly from the continued-fraction expansion of the Gaussian and (2).

(ii) τ_0 has the interpretation of the lifetime of a configuration in the ground state. The static limit takes $\tau_0 \to \infty$ or $\mathbb{F}^{(i)} = \mathbf{0}$. The net effect is then to introduce a diagonal term with a Gaussian distribution. This is the basis of the Gaussian model of Chen *et al* (1972) in the adiabatic approximation.

(iii) The term $\Sigma \, \mathbb{F}^{(i)}$ adds a diagonal term and since $\langle f^i_{n,q} \, | \, \mathbb{F} \, | \, f^i_{n,q} \rangle = -q/\tau_0$ the self-energy has a representation that is dependent on the cardinality of the basis. The same is true of the Green functions.

(iv) In analogy with the static disorder case with binary distributions, when we described excitations above the *ground state* in terms of pseudo-fermions (Mookerjee 1975), the continuous distribution case may have its excitations above the *ground state* in terms of pseudo-bosons. The energy associated with such a pseudo-boson for the Ehrenfest process is $\hbar\omega = \hbar/\tau_0$. Each time an excitation is created in the configuration space, the electron exchanges this much energy with the stochastic bath. The electron system itself (separated from the stochastic bath) is an open system in which energy is *not conserved*. The energy exchange then appears as an imaginary part of the Hamiltonian of this open system. When we model a phonon bath by an Ehrenfest bath, these pseudo-bosons are the actual phonon excitations of the lattice and $\hbar\omega$ is a quantum of energy associated with these excitations.

We have achieved a complete structural analogy between the theory for static and dynamic disorder. It is therefore a natural extension to describe the CPA for the dynamic disorder case in terms of the same delinking approximation in augmented space, as for the static case.

Figure 2 shows a part of the delinked graph in augmented space corresponding to the CPA. The same argument may now be used to determine the diagonal self-energies. The only difference is the comment (iii), which states that now the self-energies and Green functions are labelled by the cardinality of the basis functions. This is made quite apparent in the graph of figure 2, from the fact that the bubble decorations at the sites are themselves cardinality-dependent. The generalisation of (7) is then

$$\Sigma_q = -iq\hbar\omega$$

$$+ \cfrac{\lambda^2}{1/F_{q+2} + [\Sigma_{q+1} + i(q+1)\hbar\omega] - \cfrac{2\lambda^2}{1/F_{q+2} + [\Sigma_{q+2} + i(q+2)\hbar\omega] - \ldots}} \tag{12}$$

with $\Sigma(z) = \Sigma_0$ and $F_q(z) = g_{ii}(z - \Sigma_q)$. This result is identical to the result obtained by Paquet and Leroux-Hugon (1984) via a t-matrix approach, with the slight notational change: their $\Sigma_q - i\hbar\omega$ being our Σ_q. We have retained our notation as it is consistent with our earlier work on static disorder.

If we take $\tau \to \infty$ or $\omega \to 0$, (12) reduces to (7) with a Gaussian distribution, as it should. Our dynamical CPA appears as a natural generalisation of the static disorder CPA and reduces to it in this limit.
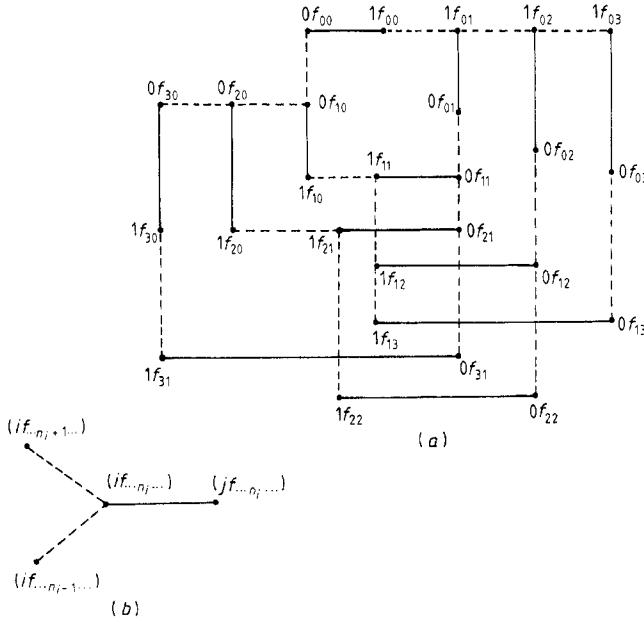
Figure 2. (*a*) Part of the check-board pattern graph for the 2CPA. Each closed loop is of length 8 and contains states of cardinality q and $q + 1$. (*b*) Tree structure after recursion is applied.

If the excitations of the stochastic bath are produced thermally, at a particular temperature T, the excitation frequency density is given by the boson distribution function

$$D(\omega) = (e^{\hbar\omega/\kappa T} - 1)^{-1}.$$

2.3. The electron–bath coupled system

As mentioned before, we may begin to describe the excitations of the ground state of the Ehrenfest bath in terms of bosons. The mathematics is very similar to that of Schultz and Shapiro (1972) and Mookerjee (1975), with boson statistics instead of fermion. If we define

$$b_i^\dagger |\ldots \gamma_n^i \ldots\rangle = (n_i + 1)^{1/2} |\ldots \gamma_{n+1}^i\rangle$$

$$b_i |\ldots \gamma_n^i \ldots\rangle = n_i^{1/2} |\ldots \gamma_{n-1}^i \ldots\rangle$$

then it is easy to see that

$$\mathbb{F}^{(i)} = -i\hbar\omega\, b_i^\dagger b_i \qquad \tilde{M}^{(i)} = \lambda(b)_i^\dagger + b_i). \tag{13}$$

In this second quantised form the augmented space Hamiltonian becomes

$$\tilde{H} = \sum \varepsilon_i a_i^\dagger a_i + \sum \sum V_{ij} a_i^\dagger a_j - i\hbar\omega \sum b_i^\dagger b_i + \lambda \sum (b_i^\dagger + b_i) a_i^\dagger a_i. \tag{14}$$

Note that the above Hamiltonian closely resembles that of a coupled electron–phonon system. The following observation is pertinent: in deriving the Hamiltonian, it was taken to be the Hamiltonian of the electrons alone. This is an open system and the

stochastic bath could exchange energy with it. Energy is not conserved and an imaginary part appeared in the electron Hamiltonian proportional to the energy exchange. If we want to compare this with the total Hamiltonian of the closed electron–phonon system, then we must replace the imaginary part with a real part $\Sigma \hbar \omega b_i^\dagger b_i$ representing the energy of the phonon excitations.

Inspection of (14) immediately shows that the model neglects the correlation between phonon amplitudes on different sites. This model is appropriate either when $T \gg T_D$ and phonons of all wavelengths are excited, so that the phonon correlation function is reasonably short-ranged, or in very dirty systems where the low-lying phonon modes are localised and the local phonon picture is not a bad one. We shall, in the application we have in mind, satisfy both these conditions.

At a temperature T then, the self-energy arising out of the coupling of the electron with the stochastic bath is (from (12)):

$$\Sigma(z) = \int d\omega \, D(\omega)\Sigma_0(z, \omega)$$

$$= \int d\omega \, D(\omega) \frac{|\lambda(\omega)|^2}{[1/F_1(z, \omega)] + (\Sigma_i + i\hbar\omega) - \dfrac{2|\lambda(\omega)|^2}{[1/F_2(z, \omega)] + \ldots}}. \qquad (15)$$

Here we have generalised (12) a little by making the coupling constant λ depend on the frequency ω as well.

Following the arguments of Paquet and Leroux-Hugon (1984), for any z there exists an integer p such that, for $q > p$, $|\Sigma_q(z, \omega)| \leq \delta$ (where δ is a preordained number, however small). This makes the recursive relations (12) and (15) tractable in practice. If we assume that $p = 1$, that is $\Sigma_q, F_{q+1} \simeq 0$ for all $q \geq 1$, then for $T \gg T_D$ we have

$$\Sigma_0(z, \omega) = |\lambda(\omega)|g_{00}(z + i\hbar\omega) \qquad \text{and} \qquad \Sigma(z) = \kappa T \int dx \, k(x)g_{00}(z + x) \qquad (16)$$

where

$$k(x) = \int d\omega \{|\lambda(\omega)|/\omega^2\}[\delta(x - \hbar\omega) + \delta(x + \hbar\omega)].$$

This is identical to the result of Girvin and Jonsson (1980) using a simple perturbative approach. The dynamic CPA is then a generalised perturbative method, in which a whole series of scattering diagrams are summed to all orders. This view of the CPA already exists in the case of static disorder (Mookerjee 1975).

If we assume that the lifetime of the stochastic bath in its *ground-state configuration*, τ_0, is much longer than the lifetimes associated with the electronic motion, we may take the energy transfer $\hbar\omega \simeq 0$. This then corresponds to the static or adiabatic limit. This gives

$$\Sigma_g(z) = \kappa T \bar{\lambda} g_{00}(z) \qquad \text{where} \qquad \bar{\lambda} = \int dx \, k(x). \qquad (17)$$

This is the standard adiabatic result.

2.4. The cluster CPA generalisation

The augmented space approach provided a tractable formulation of cluster CPA (CCPA) in the static disorder case. The generalisation provided *herglotz* Green functions at

all energies and degrees of disorder (Kumar *et al* 1982, Mookerjee *et al* 1983, 1985, Mookerjee and Yussouff 1984). Applications have been made to the density of states and conductivities in cases where there is strong scattering and the simple single-site CPA does not yield accurate results. For dynamic disorder, too, we may identify situations when it is necessary to go beyond the simple CPA described in § 2.3. The simplest situation occurs when it is necessary to take into account correlations between phonon amplitudes of adjacent sites. Cluster CPA that take these correlations into account are desirable if we wish to make quantitatively accurate calculations. Even in very dirty systems, the localised phonon modes are never localised *on a site*, but have finite extent. Generalisation beyond the single-site CPA is also desirable when the electron–phonon coupling is large.

In view of the above, let us add to the Hamiltonian a term of the type $\Sigma\Sigma\, D_{ij}b_i^\dagger b_j$ with $D_{ii} = -\Sigma\, D_{ij}$, where i and j belong to a particular cluster of neighbouring sites. If we follow a Tsukada-type cluster partitioning of the underlying lattice, the self-energy is cluster-diagonal. As before, in the CCPA the averaged Green functions $F(z)$ and the self-energies are diagonal in the cardinality-labelled partition of the configuration space. We could describe the CCPA in analogy with the static case: the closed paths that involve sites within and without the cluster and which do not lie entirely in a subspace spanned by states of the same cardinality are delinked. The delinked graphs obtained from this prescription are rather formidable and their symmetries are not immediately apparent. This is in contrast to the CPA graph whose tree-like structure allowed us with a little difficulty to obtain continued-fraction-like recurrence expressions. Figure 2(a) shows the topological structure of a part of this graph for the 2CPA. For the static case, it was shown that the t-matrix and the graphical approaches are equivalent. A very similar proof can be constructed also for the dynamical CPA. In this case we found it more convenient to follow the t-matrix approach.

The CCPA cluster t matrix is an operator in the cluster-spanned subspace $\mathbb{C}$:

$$t = [I - G(V - \Sigma)^{-1}](V - \Sigma) \tag{18}$$

where V is the random part of the Hamiltonian (in the usual t-matrix approach notation). The CCPA equations are

$$\langle f_{0,q}^{\mathbb{C}} |t| f_{0,q}^{\mathbb{C}} \rangle = 0. \tag{19}$$

The notation is consistent, with $\mathbb{C} = (i, j, k, \ldots)$ the cluster sites and $0 = (0, 0, \ldots)$ the *ground-state configuration*. Since we can also write $t = G^{-1} + [I - (V - \Sigma)G]G^{-1}$ and G^{-1} is diagonal in a cardinality-labelled partition of the augmented space, (19) is also equivalent to

$$\langle f_{0,q}^{\mathbb{C}} |[I - (V - \Sigma)G]^{-1}| f_{0,q}^{\mathbb{C}} \rangle = I. \tag{20}$$

All inverses are taken in the cluster-spanned subspaces. Note that unlike the 1CPA case the matrix $V - \Sigma$ is no longer tridiagonal in the cardinality-partitioned space. This is because, unlike the 1CPA case, there are more than one distinct configuration that have the same cardinality label. For example, in the 2CPA both the states $|f_{01,q+1}^{ij}\rangle$ and $|f_{10,q+1}^{ij}\rangle$ have the same cardinality $q + 1$, while all three of the states $|f_{02,q+2}^{ij}\rangle$, $|f_{11,q+2}^{ij}\rangle$ and $|f_{20,q+2}^{ij}\rangle$ have the same cardinality $q + 2$. Therefore the inversion in (20) is not straightforward, and must involve a recursion technique like that of Haydock *et al* (1972). Before the recursion reduces the $(V - \Sigma)G$ into a tridiagonal form, the tree-like recursive structure of the graph is not present and is the basis of the difficulty with

the graphical method. After inversion equation (20) reduces to a set of equations of the general form

$$\mathcal{R}[\Sigma_q, \Sigma_{q+1}, \dots] = I. \tag{21}$$

These are the recurrence equations giving Σ_q in terms of Σ_{q+1} and Σ_{q+2}.

Note first that the functional form of $\mathcal{R}$ is independent of the cardinality label. We should also note that since $(V - \Sigma)G$ is not symmetric in the cardinality label, we should use the non-symmetric version of the recursion technique (Haydock 1980). Moreover, if we use the argument of Paquet and Leroux-Hugon (1984) that $\Sigma_{q+p} \simeq 0$ for $p \geq p_0$, then the set of equations (21) form a closed set of recurrence relations and may be used to obtain $\Sigma = \Sigma_0$ without difficulty.

Once we have gone through the t-matrix approach, it is clear that if we use the non-symmetric recursion method of Haydock *et al* (1972) (which is essentially a change of basis) on the original chess-board pattern of figure 2(*a*), we may reduce it to a tree-like structure as shown in figure 2(*b*). Such a tree will immediately yield the recurrence relations (21) in terms of the recursion coefficients A_n, B_n and B'_n, which are themselves functions of $\Sigma_q, \Sigma_{q+1}, \dots$ and are produced during the application of recursion. All this may sound rather complicated. However, in most applications made by us and Paquet and Leroux-Hugon (1984), $\Sigma_q \simeq 0$ for $p \geq 4$, the only exceptions being for very small ω, where we may use the static limit anyway. In such cases the recursion terminates after a few steps.

2.5. Systems with both static and dynamic disorder

Putting the averaging procedure for static and dynamic disorder on the same footing was motivated by the fact that we eventually wish to study systems that have both. Highly disordered metals and dirty alloys in contact with a thermal bath are some of the systems of interest. In these, both configuration averaging over structural and compositional disorder and averaging over various *histories* of the bath are necessary. The full configuration space is a direct product of the static configuration space and the dynamic one

$$\Phi = \Phi_{st} \otimes \Phi_{dy}.$$

In general the augmented space Hamiltonian connects Φ_{gt} and Φ_{dy}. To see this clearly, we take the case of structural disorder, where the atomic potentials vary continuously depending on the varying local environments. We note that the static disorder in the atomic potentials also leads to a disorder in both τ_0 and λ. The phonon frequencies involve the electronic energy levels via the dielectric function, while the electron–phonon coupling term also involves the derivative of the electron potential. Given a distribution of the electron potential in the absence of the phonon bath, a consistent calculation of the distribution of τ_0 and λ is not an easy task, and is beyond the scope of this present work. We shall replace both τ_0 and λ by their average values. Though not explicitly stated, the work of Girvin and Jonsson (1980) also assumes this. Thus

$$\tilde{H} = \sum \tilde{M}^{(i)} B_i^{\dagger} B_i a_i^{\dagger} a_i + \sum \sum V_{ij} a_i^{\dagger} a_j - i\hbar\omega \sum b_i^{\dagger} b_i + \bar{\lambda} \sum a_i^{\dagger} a_i (b_i^{\dagger} + b_i) \tag{22}$$

where $a_i^{\dagger}$ creates an electron at the site r_i, $b_i^{\dagger}$ creates a pseudo-boson related to dynamic disorder at r_i and $B_i^{\dagger}$ creates a pseudo-boson related to static disorder at r_i.
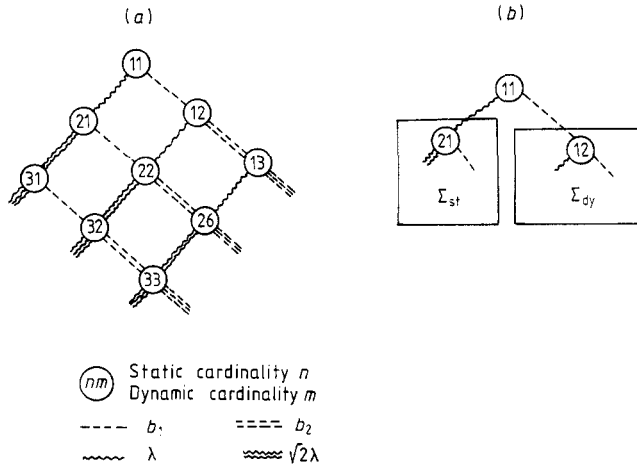
Figure 3. (*a*) Part of the delinked graph for the ICPA with both static and dynamic disorder. (*b*) Tree structure after further delinking.

In the case in which we have alloy-like static disorder, the above approximation is not a good one, and we need not average τ_0 or λ but use their two possible values τ_A, τ_B and λ_A, λ_B and the concentrations x_A, x_B of the constituents:

$$\tilde{H} = H_B + (\varepsilon_A - \varepsilon_B) \sum \sum M_{\lambda\lambda'} B^\dagger_{i\lambda} B_{i\lambda'} a^\dagger_i a_i$$

$$+ V_1 \sum \sum M_{\lambda\lambda'} a^\dagger_i a_j (B^\dagger_{i\lambda} B_{j\lambda'} + B^\dagger_{j\lambda} B_{i\lambda'})$$

$$+ V_2 \sum \sum M_{\lambda_1\lambda_2} M_{\lambda_3\lambda_4} B^\dagger_{i\lambda_1} B^\dagger_{j\lambda_3} B_{i\lambda_2} B_{j\lambda_4} a^\dagger_i a_j$$

$$+ \ldots + i\hbar(\omega_A - \omega_B) \sum M_{\lambda\lambda'} B^\dagger_{i\lambda} B_{i\lambda'} b^\dagger_i b_i$$

$$+ (\lambda_A - \lambda_B) \sum M_{\lambda\lambda'} a^\dagger_i a_i (b^\dagger_i + b_i) B^\dagger_{i\lambda} B_{i\lambda'} \tag{23}$$

where $B^\dagger_{i\lambda}$ with $\lambda = \uparrow$ or $\downarrow$ are the creation operators for pseudo-fermion excitations of the binary distribution above the *ground state* $|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \ldots \uparrow\uparrow\rangle$. In the absence of short-range order we have $M = x_A P_\lambda + x_B P_{\lambda'} + (x_A x_B)^{1/2}(T_{\lambda\lambda'} + T_{\lambda'\lambda})$, while $V_1 = V_{AA} + V_{BB} - 2V_{AB}$ and $V_2 = V_{AB} - V_{BB}$.

Let us re-examine the ICPA calculations. Figure 3(*a*) shows the relevant portions of the delinked graph in augmented space. This is related to the Hamiltonian (23), which is the easier to study at first. A glance at the graph shows that unlike the cases of pure static or dynamic disorder as in figure 1, this delinking in the case of correlated static and dynamic disorders does not lead to a tree-like structure and thus to the break-up of $\Sigma = \Sigma_{st} + \Sigma_{dy}$ with each part having continued-fraction expressions. The *square lattice* form of the full Σ in Φ allows us to obtain the self-energy by the recursion method. The continued-fraction coefficients of a square lattice can easily be generated in any reasonable computer with great facility down to several hundred steps, more than sufficient for convergence.

However, if we further decouple as in figure 3(*b*), then the tree-like structure is reintroduced and we get

$$\Sigma_{st} = a_1 + \cfrac{b_1^2}{(1/F_0) + (\Sigma_{st} - a_2) - \cfrac{b_2^2}{(1/F_0) + (\Sigma_{st} - a_3) - \ldots}}$$

$$\Sigma_{dy,q} = -i\hbar\omega q + \cfrac{|\lambda|^2}{(1/F_q) + [\Sigma_{dy,q+1} + i(q + 1)\hbar\omega] - \cfrac{|\lambda|^2}{(1/F_{q+1}) + \ldots}} \quad (24)$$

$$F_q(z) = g_{00}(z - \Sigma_{st} - \Sigma_{dy}).$$

It must be noted that this approximation *goes beyond the ICPA*. In all earlier work this kind of decoupling has been implicitly assumed. For example, if we go to the result of Girvin and Jonsson (1980), which is first-order in the dynamic part, we get for the self-energy an expression

$$|\lambda|^2 g_{00}(z - \Sigma_{st} - i\hbar\omega) = |\lambda|^2 \bar{g}_{00}(z - i\hbar\omega)$$

where the averaging over the static disorder is done *first*. This follows directly from (25), and the correlation between the static and dynamic disorder has been ignored.

3. Remarks

The methodology described above has the advantage that various types of disorder present in the Hamiltonian are treated on the same footing and their correlations may be taken into account. The augmented space technique and the graphical method of its solution ascertains that the Green functions obtained remain *herglotz*, provided we do not entertain further uncontrolled approximations. The technique allows us to go to cluster generalisations whenever these become necessary in specific situations. Further, the results reduce to established results in various limiting situations. This enhances our confidence in the proposed approximation as the generalisation of the coherent potential approximation.

One of the motivations that led us to develop the formalism is to study the conductivity of Mooij alloys (random alloys with very high residual resistivity, due to near-localisation of electrons near the Fermi level). In particular, we wish to investigate whether coupling with the phonon bath alone could provide a mechanism for low-temperature minima in the resistivity. This will be reported in a subsequent communication.

Acknowledgments

References

Bishop A R and Mookerjee A 1974 *J. Phys. C: Solid State Phys.* **7** 2161

Chen A-B, Weisz G and Sher A 1972 *Phys. Rev.* B **5** 2897
Girvin S M and Jonsson M 1980 *Phys. Rev.* B **22** 3583
Gray L J and Kaplan T 1976 *Phys. Rev.* B **14** 3462
Haydock R 1972 *PhD Thesis* University of Cambridge
—— 1980 *Solid State Phys.* **35** (New York: Academic)
Haydock R, Heine V and Kelly M J 1972 *J. Phys. C: Solid State Phys.* **5** 2845
Kaplan T and Gray L J 1982 *Excitations in Disordered Systems* (Nato ASI Series B, vol. 78) (New York: Plenum)
Kumar V, Mookerjee A and Srivastava V K 1982 *J. Phys. C: Solid State Phys.* **15** 1939
Mookerjee A 1973 *J. Phys. C: Solid State Phys.* **6** 1340
—— 1975 *J. Phys. C: Solid State Phys.* **8** 2688, 2943
Mookerjee A, Srivastava V K and Choudhry V 1983 *J. Phys. C: Solid State Phys.* **16** 455
Mookerjee A, Thakur P K and Yussouff M Y 1985 *J. Phys. C: Solid State Phys.* **18** 4677
Mookerjee A and Yussouff M 1984 *J. Phys. C: Solid State Phys.* **17** 1009
Paquet D and Leroux-Hugon P 1984 *Phys. Rev.* B **29** 593
Schultz T D and Shapiro D 1972 *Phys. Rev.* B **7** 5090
Sumi H 1977 *J. Chem. Phys.* **67** 2943