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1990 J. Phys.: Condens. Matter 2 9399

(http://iopscience.iop.org/0953-8984/2/47/014)

J. Phys.: Condens. Matter **2** (1990) 9399–9408. Printed in the UK

Conductivity in dirty systems—effect of dynamic electron–phonon coupling

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Received 17 January 1990, in final form 23 May 1990

Abstract. Using the augmented space formalism introduced previously, a dynamical cluster coherent potential is developed to study the variation of resistivity with temperature, at low temperatures, for dirty alloys whose electrons near the Fermi level are sluggish. For high enough disorder at the onset of localization we observe a minimum in the resistivity at low temperatures and an anomalous temperature coefficient of resistivity in this regime.

1. Introduction

The role played by electron–phonon coupling in determining resistivity has been studied in two limiting situations. For metallic systems with conduction electrons having a high mobility ($\rho \simeq 1$–$10\ \mu\Omega$ cm), the introduction of a thermal bath interacting with the conduction sea increases resistivity. This follows directly from the Boltzmann equation and its variational treatment leading to Mattheissen's rule: $\rho > \rho_0 + \rho(T)$, where ρ_0 is the residual resistivity. The thermal coefficient of resistivity (TCR) is always positive. In the opposite case of very dirty systems where the electrons at the Fermi level are localized, the coupling with the phonon bath actually provides a mechanism to produce non-zero conductivity. The TCR is negative (anomalous) at low temperature regimes. Intermediate in nature are the Mooij alloys with $\rho \simeq 150$–$600\ \mu\Omega$ cm whose sluggish conduction electrons have very low mobility (Mooij 1973). These also exhibit negative TCR at low temperatures. In such systems the Boltzmann formalism with its weak scattering basis breaks down. Girvin and Jonsson (1980, hereafter called GJ) first introduced a theoretical basis which spans the Boltzmann and the hopping conduction regimes. The mechanism on which these authors focused was the ability of the sluggish conduction electrons to exchange energy with the phonon bath, leading to an increase in conductivity, and not one which relied on any special features of the density of states or static structure factors. GJ correctly expressed reservations about the earlier CPA treatments (Chen *et al* 1972, Brouers and Brauwers 1975) on two grounds. First, the necessary adiabatic approximation breaks down, because the sluggish electrons spend a time near a vibrating ion core of the same order of magnitude as the inverse frequency with which the ion vibrates. We cannot decouple the electron and the phonon degrees of freedom. The static CPA was shown by this author (Mookerjee 1990, referred to as I), to correspond exactly to the adiabatic approximation. Secondly, in these dirty alloys we are in a strong scattering regime where the CPA is itself incapable of predicting the onset of localization (sluggishness) (Haydock and Mookerjee 1974).

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Recently this author has introduced a *dynamical* CPA (see I) based on the augmented space formalism first introduced for static disorder problems (Mookerjee 1973). The dynamical CPA treats the electronic and the thermal bath degrees of freedom on the same footing and enables us to go beyond the adiabatic approximation. In case the characteristic times associated with the different degrees of freedom are on very different scales, this dynamical CPA was demonstrated to be equivalent to various expressions earlier obtained by Sumi (1974) and Girvin and Jonson. In this communication we shall focus on systems with sluggish electrons in the vicinity of the Fermi level. We shall further modify the dynamical CPA to include the contribution of the so-called maximally crossed diagrams in order to introduce features which revalidate the modified approximation in the regimes near the onset of localization (Economou 1983, Chitnavis 1985).

The aim of this communication is to improve upon the ideas of GJ in two specific aspects. First, GJ treated the dynamical disorder within a perturbation approach while the static disorder was treated *exactly* numerically on a Bethe lattice. The assumption made, though not explicitly stated, was that the effects of the static and dynamic disorder were uncorrelated. The last assumption was shown in I to be invalid in specific examples. We shall treat both the static and dynamic disorder on the same footing. Second, the modification of the CPA to include the maximally crossed diagrams will allow us, in conjunction with the recursion method of Haydock *et al* (1972), to treat conductivity on realistic lattices (Mookerjee *et al* 1985, Mookerjee 1986) and avoid the less convincing estimates of the vertex term of GJ on Cayley trees and the tedious Monte Carlo justifications.

2. Conductivity and TCR

We shall study the effect of a thermal bath on the conductivity of dirty systems in the strong scattering regime. These systems have resistivities in the range 150–600 $\mu\Omega$ cm and, in the absence of the phonon bath, the electronic states near the Fermi level have very low mobilities. These sluggish electrons are characterized by timescales τ_e related to their lifetimes in the vicinity of a particular ion and $\tau_e \simeq O(\tau_0)$, where τ_0 is the timescale associated with the bath ground state. The adiabatic approximation breaks down and our dynamical disorder method comes into its own. In the strong scattering regime, near Anderson localization, the Boltzmann formalism also breaks down and we shall use the Kubo formalism to go further.

Suppose that at a time t the electron is localized about an ion situated at r_i. After a time τ_0, in the presence of a bath, the configuration may have changed to one which allows the electron to leak out. Our arguments would suggest that as long as $\tau_0 \geqslant \tau_e$, the coupling with the phonon bath may enhance conductivity in some temperature ranges. This is the mechanism we wish to study.

We should note, however, that in any concrete example there may be other mechanisms which enhance conductivity, like special features of the density of states at the Fermi level (Chen *et al* 1972), interband transitions (Allen and Chakraborty 1978) or Kondo-like tunnelling (Tsuei 1978, Black and Gyorffy 1978). There is no *a priori* argument to suggest which of these mechanisms is dominant. In this application we shall not look at these mechanisms, but rather shall choose a model in which these are absent. The model will be a simple tight-binding model with one orbital per site. The density of states will be featureless with the Fermi level situated at the band centre where the density of states has a very weak energy dependence. The generalization to many-orbital

models has been discussed by Chitnavis and Raghavan (1983) and Mookerjee *et al* (1985).

As we have stated before, the use of the simple CPA to describe conductivity in situations near the Anderson transition is not valid. The CPA yields erroneous information in such regimes (Haydock and Mookerjee 1974), and grossly overestimates the mobilities. Generalization to cluster CPAs improves matters (Mookerjee *et al* 1985, Mookerjee 1986) but as we are still unable to take into account large clusters, they overestimate mobilities. To adequately treat sluggish electrons we have to improve our approximation to include the effect of the whole class of the so-called maximally crossed diagrams (Langer and Nèel 1966, Abrahams *et al* 1979). We discuss this generalization within the augmented space formalism. Recently, Chitnavis (1985) reported a similar work based on the so-called travelling cluster approximation (TCA) of Mills and Ratanavararaksa (1978), which is also based on our augmented space technique. In the static part of the augmented space this has similarities with our approach, but differs in specific details of approximation.

The basis of our approach is the Kubo expression:

$$\sigma^{\alpha\beta} = \int_{-\infty}^{\infty} \mathrm{d}E\,(-\partial f/\partial E)[S^{\alpha\beta}(E^+, E^+) - S^{\alpha\beta}(E^+, E^-)]_{\mathrm{av}} \tag{1}$$

with

$$S^{\alpha\beta}(E_1, E_2) = \langle j^\alpha; j^\beta \rangle.$$

The term with $E_1 = E_2 = E^+$ is related to the particle–particle propagator, whereas the term with $E_1 = E_2^* = E^+$ is related to the particle–hole propagator.

By definition:

$$\langle \boldsymbol{A}; \boldsymbol{B} \rangle = (\mathrm{i}\hbar/\pi)\ \mathrm{Re\ Tr}\, \boldsymbol{A}\boldsymbol{G}(E_1)\boldsymbol{B}\boldsymbol{G}(E_2)$$

where $\boldsymbol{G}$ is the one-particle propagator, while the current term is defined by:

$$j^\alpha(k) = (e/\hbar)\nabla^\alpha \boldsymbol{H}_0(k). \tag{2}$$

Here $f(E)$ is the Fermi distribution function and $\boldsymbol{H}_0$ is the translationally symmetric part of the Hamiltonian.

The calculation of the configuration average of quantities like $S^{\alpha\beta}(E_1, E_2)$ has been discussed in detail within the CCPA by Mookerjee *et al* (1985). Generation of scattering diagrams within the augmented space approach for the two-particle Green function has been discussed earlier (Mookerjee 1975b, 1976). A careful study of the topology of the scattering diagrams reveals that the dominant correction due to randomness in the current term arising from the off-diagonal disorder is a replacement of the undressed current j^α by a renormalized current $\boldsymbol{J}^\alpha$ (Mookerjee 1986) given by:

$$\boldsymbol{J}^\alpha(E_1, E_2) = \boldsymbol{j}^\alpha + \xi^\alpha(E_1) + \xi^\alpha(E_2) + I(E_1, E_2)\delta\xi^\alpha(E_1)$$

$$I(E_1, E_2) = \int \frac{\mathrm{d}^3\boldsymbol{k}'}{8\pi^3}\,\delta\Sigma(\boldsymbol{k}', E_2(\bar{G}(\boldsymbol{k}', E_2) \times \left(\int\int \frac{\mathrm{d}^3\boldsymbol{k}'\,\mathrm{d}^3\boldsymbol{k}''}{8\pi^3\,8\pi^3}\,\delta\Sigma(\boldsymbol{k}', E_1)\delta\Sigma(\boldsymbol{k}'', E_2)\delta\bar{G}(\boldsymbol{k}', E_1)\delta\bar{G}(\boldsymbol{k}'', E_2)\right)^{-1/2}. \tag{3}$$

Here $\bar{G}(\boldsymbol{k}, E)$ is the configuration averaged one-particle propagator, $\Sigma(\boldsymbol{k}, E)$ is the self-energy defined via the relation $\bar{G} = (E\boldsymbol{I} - \bar{\boldsymbol{H}} - \boldsymbol{\Sigma})^{-1}$ where $\bar{\boldsymbol{H}}$ is the configuration average of the Hamiltonian. In all applications either $E_1 = E_2^* = E^+$, in which case the operator

δ is $-\mathrm{Im}$[e.g. $\delta\Sigma = -\mathrm{Im}\,\Sigma$]; or $E_1 = E_2 = E^+$, in which case δ is $\partial/\partial E$ [e.g. $\delta\Sigma = \partial\Sigma/\partial E$].

The calculation for $\xi^\alpha(\boldsymbol{k}, E)$ is closely related to that of the self-energy and has also been described in detail in the earlier work referred to for J^α. The remainder of the correction involves a vertex-like term which is derived via the Ward identity from $\Sigma(z)$.

The term $[S^{\alpha\beta}(E_1, E_2)]$ can be broken up into four distinct contributions: the Ziman–Drude term $[S_0^{\alpha\beta}(E_1, E_2)]$; the two contributions from the vertex corrections, one coming from the CPA scattering diagrams and the other from the related maximally crossed diagrams; and the remainder. In our approximation we shall neglect the last contribution.

Let us now introduce the various two-particle propagators and vertex terms we shall use in our subsequent derivations and the relations between them. Unfortunately, the literature does not follow a consistent notation for these, so an initial definition is pertinent:

$$[S^{\alpha\beta}(E_1, E_2)] = \sum_{mn}\sum_{pq} J^\alpha_{mn} G^{\mathrm{II}}_{mn,pq}(E_1, E_2) J^\beta_{pq}. \tag{4a}$$

G^{II} is the two-particle propagator and J^α is the renormalized current term already defined. If we define $g^{\mathrm{II}}(E_1, E_2)$ as the free two-particle propagator $\bar{G}(E_1) \otimes \bar{G}(E_2)$, then the vertex correction Γ is defined as

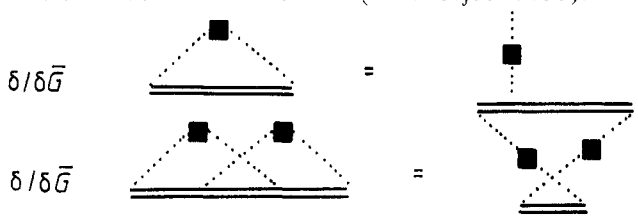
$$G^{\mathrm{II}}_{mn,pq} = g^{\mathrm{II}}_{mn,pq} + \sum_{ij}\sum_{kl} g^{\mathrm{II}}_{mi,pj}\Gamma_{ij,kl} g^{\mathrm{II}}_{kn,lq}. \tag{4b}$$

While the scattering vertex Λ is defined as:

$$G^{\mathrm{II}}_{mn,pq} = g^{\mathrm{II}}_{mn,pq} + \sum_{ij}\sum_{kl} g^{\mathrm{II}}_{mi,pj}\Lambda_{ij,kl} G^{\mathrm{II}}_{kn,lq}. \tag{4c}$$

The vertex correction Γ is related to the self-energy Σ via the Ward identity $\Gamma = \delta\Sigma/\delta\bar{G}$ (Mookerjee 1976). We may easily check this diagrammatically if we read $\delta/\delta\bar{G}$ to be the operation of removing a $\bar{G}$ line from the diagrams for Σ, without breaking up the diagrams into two or more unconnected bits (Mookerjee 1975b).

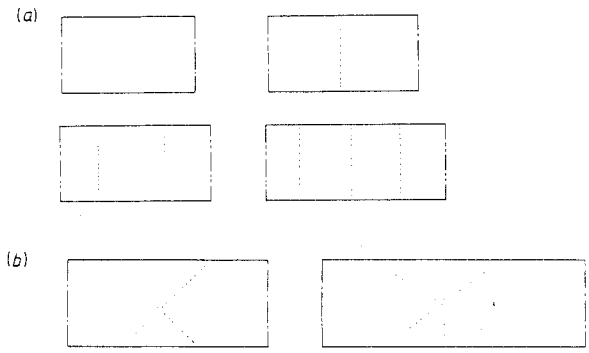
e.g.



The CPA ladder diagrams for the averaged two-particle Green functions $[S^{\alpha\beta}(E_1, E_2)]_{\mathrm{av}}$ with the renormalized currents are shown in figure 1(a) and the corresponding maximally crossed diagrams are shown in figure 1(b). We shall now consider an approximation for Γ involving contributions *only* from the 1 CPA ladder diagrams of figure 1(a) and the corresponding maximally crossed diagrams of figure 1(b). We have

$$\Gamma \simeq \Gamma^{\mathrm{CPA}} + \Gamma^{\mathrm{cr}}. \tag{5a}$$

Using the equations (4a–c) and looking at the scattering diagrams we can easily see that the CPA contribution to Γ can be written in terms of a single-site scattering vertex λ_i e.g. for the binary disorder problem $= c_A c_B(\varepsilon_A - \varepsilon_B)^2\delta_{ij}$. Diagrammatically we have

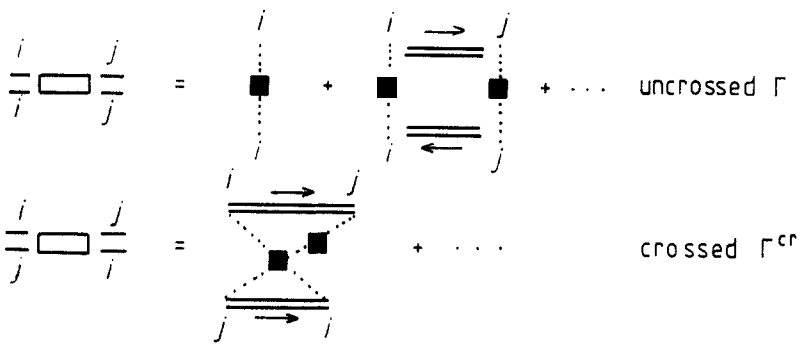


where the scattering lines represent all possible augmented space diagrams:

Figure 1. (*a*) CPA ladder diagrams for the two-particle Green function. (*b*) The corresponding maximally crossed diagrams.

$$\Gamma^{\mathrm{CPA}}_{ii,jj} = \lambda_i \delta_{ij} + \lambda_i \sum_k g^{\mathrm{II}}_{ik,ik} \Gamma_{kk,ij}. \tag{5b}$$

Looking at the scattering diagrams for Γ:



$\Gamma^{\mathrm{cr}}_{ij,ji}(E_1, E_2)$ may be directly related to its *uncrossed* CPA counterpart $\Gamma_{ii,jj}(E_1, E_2)$ by the relation

$$\Gamma^{\mathrm{cr}}_{ij,ji}(E_1, E_2) = \Gamma^{\times}_{ii,jj}(E_1, E_2^*) \tag{5c}$$

where the uncrossing operation $\times$ on any separable operator of rank 4 may be defined as follows:

$$\boldsymbol{A}(E_1, E_2) = \boldsymbol{a}(E_1) \otimes \boldsymbol{b}(E_2) \quad \text{so that} \quad A_{ij,km} = a_{ik}(E_1) b_{jm}(E_2)$$

then

$$A^{\times}_{ij,km} = a_{i,j}(E_1) b_{mk}(E_2^*). \tag{5d}$$

We note that the particle–hole vertex diagram is related by the uncrossing operation to the particle–particle vertex diagram and vice versa.

The contribution of the crossed diagrams may also be written:

$$\Gamma^{\mathrm{cr}}_{ij,ji} = \lambda_i \hat{g}^{\mathrm{II}}_{ij,ji} \lambda_j + \lambda_i \sum_k \hat{g}^{\mathrm{II}}_{ik,ki} \Gamma^{\mathrm{cr}}_{kj,jk} \tag{5e}$$

where $\hat{g}^{\mathrm{II}}_{ij,ji} = \bar{G}_{ij} \bar{G}_{ji} (1 - \delta_{ij})$. The exclusion of $i = j$ terms are necessary so as not to

double-count contributions between (5*b*) and (5*e*). Taking Fourier transforms in (5*e*) we obtain the following:

$$\Gamma^{\mathrm{cr}}(k, E_1, E_2) = \frac{\lambda^2 v(k, E_1, E_2)}{1 - \lambda v(k, E_1, E_2)}. \tag{6a}$$

Here,

$$u(k, E_1, E_2) = \int \frac{\mathrm{d}^3 k'}{8\pi^3} \bar{G}(k', E_1)\bar{G}(k - k', E_2) \tag{6b}$$

$$v(k, E_1, E_2) = u(k, E_1, E_2) - F(E_1)F(E_2) \tag{6c}$$

$$F(E) = \bar{G}_{ii}(E).$$

The contribution of the vertex correction coming from the crossed diagrams to $S^{\alpha\beta}$ may be written as

$$\begin{aligned} [S^{\alpha\beta}(E_1, E_2)]^{\mathrm{cr}}_{\mathrm{av}} &= \sum_i \sum_j Q^{\alpha}_{ij}(E_1, E_2)\Gamma^{\mathrm{cr}}_{ij,ji}(E_1, E_2)Q^{\beta}_{ji}(E_1, E_2) \\ Q^{\alpha}_{ji}(E_1, E_2) &= \sum_k \sum_m \bar{G}_{jk}(E_1)J^{\alpha}_{km}(E_1, E_2)\bar{G}_{mi}(E_2)(1 - \delta_{ij}). \end{aligned} \tag{6d}$$

Taking Fourier transforms and substituting into (6*d*) from (6*a*), (6*b*) and (6*c*) we obtain

$$\begin{aligned} [S^{\alpha\beta}(E_1, E_2)]^{\mathrm{cr}}_{\mathrm{av}} = \int\int \frac{\mathrm{d}^3 k\, \mathrm{d}^3 k'}{8\pi^3 8\pi^3} J^{\alpha}(k, E_1, E_2)J^{\beta}(k', E_2, E_1) \ldots \\ \Gamma^{\mathrm{cr}}(k + k', E_1, E_2)\bar{G}(k, E_1)\bar{G}(k, E_2)\bar{G}(k', E_1)\bar{G}(k', E_2). \end{aligned} \tag{6e}$$

The contribution of the second term on the right-hand side of (6*c*) vanishes in the 1 CPA single-orbital model, as does the vertex contribution of the ladder CPA diagrams. In the multi-orbital case both terms lead to spurious infrared divergences which may be eliminated by correctly taking the thermodynamic and static limits (Chitnavis and Raghavan 1983).

The Ziman–Drude term is:

$$[S_0^{\alpha\beta}(E_1, E_2)] = \int \frac{\mathrm{d}^3 k}{8\pi^3} J^{\alpha}(k, E_1, E_2)J^{\beta}(k, E_1, E_2)\bar{G}(k, E_1)\bar{G}(k, E_2). \tag{7}$$

It is instructive to replace (6) and (7) back into (1) and obtain the weak scattering limit at low temperatures. To do this we change the variables in (6*e*) to $K = k + k'$ and $K' = k - k'$ and expand $u(K, E_1, E_2)$ about $K = 0$. Keeping only the leading term in K^2 we may integrate out the K variable using an upper cut-off of K as K_0 which is of the order of the inverse of the localization radius of the electron.

$$\begin{aligned} \sigma &\simeq (e^2\hbar^2/4\pi)\{\mathcal{J}(E_{\mathrm{F}})/|\mathrm{Im}\,\Sigma(E_{\mathrm{F}})| - (1/8\pi^3)K_0\} \\ \mathcal{J}(E) &= \int \frac{\mathrm{d}^3 k}{8\pi^3} |\nabla_k H_0(k)|^2 \delta[E - H_0(k)]. \end{aligned} \tag{8}$$

This is the correct form of the weak scattering limit with the crossed vertex correction (Economou 1983).

We shall now introduce the effects of dynamical disorder within the augmented space technique as described in a previous work (I). We augment the Hilbert space $\mathcal{H}$ in which the Hamiltonian of the electron is described by another Φ_{dy} on which the thermal degrees

of freedom are described. The augmented Hamiltonian is now constructed as described in I in some detail. We are modelling the thermal bath by an Ehrenfest bath, the simplest bath with a non-trivial memory function. We are interested only in qualitative aspects of dynamical disorder. More complicated baths like, e.g. the semi-Markov bath, have been described in some detail in the thesis of Paquet (1964).

$$\mathbf{H} = H_0 \otimes I + \sum [\lambda \mathbf{M}^{(i)} \otimes P_i + i\hbar F^{(i)}]$$

with $\mathbf{M}^{(i)} = I \otimes I \otimes \ldots \otimes M_i \otimes \ldots \otimes I$

$$F^{(i)} = I \otimes I \otimes \ldots \otimes F_i \otimes \ldots \otimes I. \tag{9}$$

The representation of M_i is tridiagonal with $a_n = 0$ down the diagonal and $b_n = n$ down the off-diagonal positions, while F_i are diagonal with eigenvalues $-n/\tau_0$. In analogy with the static disorder case, any configuration average may be written as:

$$[\mathcal{F}(H)] = \langle f|\mathcal{F}(\mathbf{H})|f\rangle \tag{10}$$

where $|f\rangle = \Pi^{\otimes} |\gamma_0^i\rangle |\gamma_0\rangle$ has a representation $\gamma^*(r)$ which is the stationary solution of the Fokker–Planck equation:

$$\nabla \cdot [v(r)\gamma(r)] + \tfrac{1}{2}\nabla^2[d(r)\gamma(r)] = 0. \tag{11}$$

$v(r)$ and d(r) are the local velocity and diffusion constant terms.

Since both $M^{(i)}$ and $F^{(i)}$ are functions of the cardinality n, the self-energies, the Green functions and the vertex functions related to response functions are all cardinality-dependent. The concept of cardinality, i.e. the number of applications of the Hamiltonian needed to obtain the given state from the so-called ground state, has been discussed earlier (I). Paquet and Leroux-Hugon has described in some mathematical detail the modification of equations (4)–(6) in the presence of cardinality-dependent augmented space, characteristic of the Ehrenfest bath. We shall quote here their pertinent results.

In the absence of cardinality dependence we obtain from (4a) and (4b) the relationship between the vertex correction Γ and the scattering vertex Λ as

$$\Gamma = (I - \bar{G}\bar{G}\Lambda)^{-1}\Lambda. \tag{12a}$$

Equation (4b) is modified to give

$$\begin{aligned} G^{\mathrm{II}(n)} = {} & g^{\mathrm{II}(n)} + g^{\mathrm{II}(n)} \sum_q \Gamma^{(n,q)}\, g^{\mathrm{II}(n+1)} \\ & - g^{\mathrm{II}(n)} \sum_q \Gamma^{(n,q)} [F^{(n+q)} R^{(n+q)} \otimes F^{(n+q)} R^{(n+q)} g^{\mathrm{II}(n+q)} \\ & - F^{(n+q)} R^{(n)} \otimes F^{(n+q)} R^{(n)} g^{\mathrm{II}(n)}] \end{aligned} \tag{12b}$$

where

$$\begin{aligned} & F^{(n)}(z) = G_{ii}^{(n)} \quad \text{and} \quad R^{(n)}(z) = [G^{(n)}(z)]^{-1} \\ & \Gamma^{(n,q)} = [1 - \sum_p G^{(n+p)} \otimes G^{(n+p)} \Lambda^{(n,p)}]^{-1} \Lambda^{(n,p)}. \end{aligned} \tag{12c}$$

This is a generalization of (12a) and the scattering vertex $\Lambda^{(n,q)}$ is given by Paquet and Leroux-Hugon (1984) (equations (49)–(51) and (75)) in terms of the cardinality dependent t-matrices:

$$\Lambda^{(n,q)} = t^{n,n+q} \otimes t^{n+q,n}. \tag{12d}$$

The second term in (12b) describes correlated propagation of two particles, both of them

experiencing one disorder excitation, while the third term corresponds to the difference between propagation of two particles in the presence and absence of disorder excitations. In the absence of dynamic disorder (or in the static limit) this last term vanishes. This non-local term arises because two electrons at different times, on the same site, have their scatterings correlated if the time lapse between two collisions is smaller than the correlation time of the potential at that site. For very fast dynamics, the second term also becomes negligible, since the particles are not affected by the noise bath and move in an uncorrelated manner.

As in the case of single-particle propagators (described in I), equation (12) shows that calculations of two-particle propagators are also in the form of recurrence relations which converge within a finite number of iterations in the regimes of interest.

This formulation has several advantages. Firstly, it circumvents the usual difficulties with the CPA methods in describing sluggish electrons by incorporating the crossed diagrams. Secondly, in this particular form it is unnecessary to perform the complicated Monte Carlo simulations of GJ to obtain reasonable qualitative results. Furthermore it is unnecessary to restrict ourselves to Cayley tree lattices. All the Green functions and vertices may be easily obtained within the augmented space formalism for any realistic lattice by using the recursion method of Haydock *et al* (1972). The vertex terms which concern us may be obtained from the self-energies through the Ward identities. The estimates of GJ provide us with a valuable background against which to compare our work.

3. Results and discussion

We present here a calculation of the resistivity based on the preceding formulation and a simple, non-trivial model: a tight-binding Anderson model with one orbital per site on a simple cubic lattice with only diagonal disorder. The Hamiltonian may be written as

$$\mathbf{H} = \sum \varepsilon_i |i\rangle\langle i| + \sum \sum V_{ij} |i\rangle\langle j| \tag{13a}$$

with V_{ij} being non-random and non-zero only between nearest neighbours. The diagonal elements ε_i are random and independently and identically distributed. We have chosen a semi-elliptic distribution to facilitate the calculations:

$$P(\varepsilon_i) = (2/\pi W^2)(W^2 - \varepsilon_i^2)^{1/2}. \tag{13b}$$

W is the half-band width and the disorder parameter is defined as the ratio $d = |W/2ZV|$, where $Z = 6$ is the number of nearest neighbours. It is interesting to note that neither the shape of the distribution nor the lattice has any qualitative effect on the results.

We first calculate the self-energy within the CPA using both static and dynamical disorders, with the model electronic system in contact with an Ehrenfest bath. We have assumed that the Fermi level lies at the centre of the band. For the cubic lattice the band centre has no special features. The above choice is aimed at eliminating from our results any effect due to special features of the density of states at the Fermi level. Note, however, that the formalism does not require this assumption and remains equally tractable for any other choice.

Figure 2 shows the plot of $\ln \rho$ against the self-energy for various degrees of disorder. For small disorders, the conduction electrons at the Fermi level are extended and the Ziman–Drude term dominates. In this regime Mattheissen's rule is satisfied and the resistivity increases with temperature, giving rise to a positive TCR. For higher values of

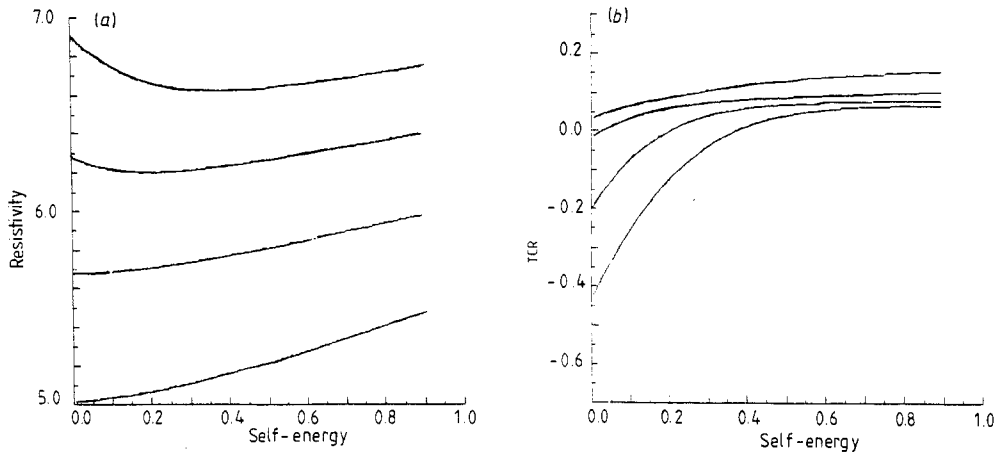


Figure 2. (*a*) The log of resistivity against the self-energy due to dynamical disorder, for increasing disorder $W/B = 5, 7, 9, 11$, where W is the width of variation of the ϵ values and B the bandwidth. (*b*) The thermal coefficient of resistivity (TCR) against the self-energy for the same four samples. Note that we have assumed that the total self-energy is the sum of self-energies due to the static and dynamical disorder.

disorder, the conduction electrons at the Fermi level are sluggish, giving rise to a very high residual resistivity. In the low-temperature regime these systems show the characteristic minimum in the resistivity and an anomalous negative TCR. This behaviour of the resistivity is qualitatively very similar to that of Girvin and Jonsson (1980). The quantitative numerical differences may arise because of the different estimates of the vertex correction in the two papers. This difference has been discussed earlier (paper I).

The above model serves to isolate the effect of dynamical disorder in giving rise to resistivity minima at low temperatures. In realistic Mooij alloys the formalism has to be modified, taking into account the various features discussed earlier in the text. The origin of the anomalous TCR may also not be unique but rather a combination of various effects already discussed. Our formalism, wedded to the recursion method, provides a powerful tool for microscopic study of such alloys.

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