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Dynamical electron-phonon interaction and conductivity in strongly disordered metal alloys

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A theory of transport in random metal alloys is presented which focuses on certain model-independent features of the electron-phonon dynamics which have been previously neglected. It is found that in the low-resistivity limit the adiabatic-phonon approximation is valid and the disorder associated with phonons increases the resistivity. In the high-resistivity limit where the weak-scattering approximation breaks down due to incipient Anderson localization, the adiabatic-phonon assumption also fails, and phonons actually assist the mobility, producing an anomalous negative temperature coefficient of resistivity. Model analytical and numerical calculations suggest that this mechanism could be the source of the Mooij correlation between the resistivity and its temperature coefficient. The connection between these results and recent scaling theories of localization is discussed.

I. INTRODUCTION

In recent years experiments on strongly disordered metal alloys and other poorly conducting metals have revealed a wealth of interesting transport properties which defy explanation by the conventional transport theory that has been so successful in applications to good metals. Of particular interest is the discovery by Mooij[1] of a correlation between the temperature coefficient of resistivity (TCR) and the resistivity of metallic systems. Mooij found that metals with resistivities less than $\rho^* \sim 150\ \mu\Omega$ cm tend to have the usual positive TCR, while most alloys with resistivities greater than ρ^* are anomalous in that over a large temperature range they have negative TCR's. This correlation is quite universal, holding for a wide variety of both glassy and crystalline random metal alloys.

Similar anomalies have been reported for the thermoelectric power[2] and the magnetoresistance.[3] In the latter case a particularly interesting observation is that systems with negative TCR tend to exhibit negative magnetoresistance. Another anomaly which has attracted considerable attention[4-6] is the fact that the resistivities of the A 15 compounds do not increase linearly with temperature and structural damage but rather tend to saturate at approximately ρ^*, the same resistivity appearing in the Mooij correlation.

Numerous mechanisms and theories have been proposed to explain these anomalies in nonmagnetic alloys including a generalized Ziman theory,[7-11] the Mott s-d scattering model,[12,13] a Kondo-type mechanism involving two-level tunneling states,[14,15] theories which study the interference between phonon and impurity scattering mechanisms,[16-21] and a theory which generalizes the Boltzmann equation to include interband transitions.[22] Under the appropriate circumstances, each of these theories can explain some of the observed transport anomalies. The extended Ziman theory in particular has been remarkably successful, but all these theories are rather specific; that is, they depend for their sucess on special features in the density of states, the static structure factor, etc. In addition, the theories to data have generally made some sort of weak-scattering approximation. This seems unreasonable since the metals in question are sufficiently dirty so that they have very small electronic mean free paths.

It is important to ask what new and fundamental physical phenomena are intrinsic to highly disordered conductors. With this in mind, we have recently[23] discussed the problem of transport anomalies from a point of view which is valid in the extreme dirty limit and pointed out certain universal features of the electron-phonon dynamics which appear in this limit and which could be the source of the Mooij correlation. The purpose of the present paper is to extend our initial discussion and to provide more details of the numerical calculations reported earlier.

The organization of the remainder of the paper is as follows. Section II discusses the failure of the weak-scattering picture and the role of the breakdown of the adiabatic-phonon approximation. Sections III, IV, and V introduce the model and the method of calculation. Sections VI and VII discuss the analytical and numerical results, respectively. Sec. VIII summarizes the present work, while its relation to recent scaling theories of localization in random systems is discussed in the Appendix.

II. BREAKDOWN OF THE WEAK-SCATTERING PICTURE

It is not difficult to demonstrate the failure of conventional transport theory in highly disordered metals. In fact the Mooij correlation is *inconsistent with the Boltzmann equation formalism itself.*

The central quantity in the present discussion is the temperature coefficient of resistivity

$$\alpha \equiv \frac{d \ln \rho(T)}{dT} . \tag{2.1}$$

In most metals α is positive because phonon scattering decreases the electronic mean free path as the temperature is raised. The sign of α can be deduced from Matthiessen's rule which asserts that the total resisitivity in the presence of two (or more) scattering mechanisms is equal to the sum of the resistivities that would result if each mechanism were the only one operating, i.e.,

$$\rho = \rho^{(1)} + \rho^{(2)} . \tag{2.2}$$

Matthiessen's rule as stated in Eq. (2.2) follows from the Boltzmann equation with the assumption of a wave-vector-independent relaxation time for each scattering mechanism.[24] If ρ_0 is the resistivity of a disordered metal at zero temperature and $\rho_{\text{ph}}(T)$ is the resistivity of the *pure* (ordered) metal due to electron-phonon scattering, then the resistivity of the disordered metal at finite temperatures as given by Matthiessen's rule is

$$\rho(T) = \rho_0 + \rho_{\text{ph}}(T) . \tag{2.3}$$

It follows from Eq. (2.3) that $\rho(T) \geq \rho_0$ and that the TCR is positive ($\alpha > 0$).

Most "good" metals to some extent obey Matthiessen's rule and typically have $\rho \sim 1-10$ $\mu\Omega$ cm and $\alpha \sim 300-600$ ppm/K. However, as Mooij has pointed out, there exist many highly disordered metals which are poor conductors ($\rho \sim 100-600$ $\mu\Omega$ cm) and have $\rho(T) \leq \rho_0$ and *negative* TCR's ($\alpha < 0$). These materials clearly violate Mattheissen's rule.

If the relaxation-time approximation is abandoned, Eq. (2.2) no longer holds. However, there exists a variational principle for the Boltzmann equation from which one can show rigorously that[24]

$$\rho \geq \rho^{(1)} + \rho^{(2)} . \tag{2.4}$$

The highly disordered alloys with $\rho(T) \leq \rho_0$ necessarily violate even this inequality. This means that the *Boltzmann-equation formalism itself is breaking down.* Apparently what is happening is that, because of the strong disorder and resulting multiple correlated scattering, the Boltzmann *hypothesis* of independent scattering events fails. There must exist some sort of "interference" between the impurity and phonon scattering mechanisms which is capable of producing the negative TCR observed in highly disordered metals.

The Ziman theory invokes this interference by considering (in low-order perturbation theory) coherent scattering between pairs of atoms. We are proposing an additional rather general mechanism involving a breakdown of the usual static-phonon approximation due to incipient localization. In the limit of Anderson localization, this mechanism passes continuously into the phenomenon of phonon-assisted hopping.

We begin a discussion of this mechanism by recalling that Mott[25] has suggested from dimensional arguments that there exists a maximum metallic resistivity which for a three-dimensional system with lattice constant a is ha/e^2. For $a = 3$ Å this is 60 $\mu\Omega$ cm. Detailed calculations[25] indicate that ρ_{max} may be more on the order of 1000 $\mu\Omega$ cm. These considerations suggest that the alloys with anomalous transport properties are sufficiently dirty so that they are approaching the maximum metallic resistivity and therefore are not far from Anderson localization. Hence perturbation theory breaks down and the simple picture of weak scattering is not valid. Presumably, the coherent scattering from large clusters that eventually induces localization is already important. In this strong-scattering regime the electrons should be thought of as diffusing around rather slowly or (in the extreme limit) as hopping between quasilocalized states rather than being occasionally scattered between nearly coherent plane-wave states.

If the disorder is so large that the time spent around a particular ion by a diffusing electron is on the order of the characteristic time for ionic motion, the usual adiabatic- (or static-) phonon approximation breaks down, and the dynamical electron-phonon interaction (as will be shown) causes the mobility to increase rather than decrease with temperature. This is known to occur for localized states (in the form of phonon-assisted hopping), but *we are proposing that it occurs even before localization is reached.* In the opposite limit of low resistivity, the additional disorder associated with the phonons causes the mobility to decrease with temperature. Hence this mechanism, which works for both crystalline and glassy materials, is consistent with the Mooij correlation and is quite universal in that it relies solely on the ability of the phonons to exchange energy dynamically with the electrons and does not require any special features in the density of states, etc. Thus this effect, which has to date been neglected, should be present in every case, although it will not necessarily dominate over the mechanisms which have been previously proposed.

The effect of phonons on the conductivity has been previously considered within the framework of the coherent potential approximation (CPA).[18,19] There are two problems with this. First, the CPA is not valid in the dirty limit because it does not predict Anderson localization,[26] and second, in order to apply the CPA, it is necessary to make the adiabatic-phonon approximation (this approximation is also made in the Ziman theory). Chen, *et al.*[18] argue that the ionic motion is slow so that one may assume that the phonon coordinates are static, Gaussian-distributed random variables. They further argue that in the dirty limit where the mean free time is small, the uncertainty in the electron energy is large compared to the maximum phonon energy so that the conservation of energy in the scattering of one electron by one phonon is of little consequence. Such uncertainty-principle arguments may work well in some cases[27] but are dangerous since they are definitely wrong for the case of strong disorder. As will be seen from our model calculation, the adiabatic-phonon approximation does indeed work well in the low-disorder limit. However, in the dirty limit the electrons are diffusing so slowly that they are sensitive to the time dependence of the phonon amplitudes. Thus the adiabatic approximation gets worse with increasing disorder, not better. It is the dynamics associated with this breakdown of the adiabatic approximation which leads to phonon-assisted mobility.

Chen *et al.* obtain an interference between (static) phonons and the impurity potential which they suggest represents phonon-assisted hopping. However, no phonon dynamics is involved, and the interference arises solely because of sharp structure in the density of states near the Fermi level. While this may actually be present in some systems, this is not the dynamic effect we are seeking, and we specifically avoid it by choosing a model with minimal structure in the density of states.

In order to overcome the objections to the CPA and the adiabatic-phonon approximation, one would like to find a scheme for calculating the conductivity which is valid in the dirty limit and in which phonon dynamics can be included. Such a scheme is outlined in the next three sections.

III. THE MODEL

In order to study electron-phonon dynamics and transport properties in poorly conducting metals, we consider a model system described by a simple tight-binding Hamiltonian with random-site energies and coupling to local phonon modes of the form

$$H=t\sum_{i\delta} c^{\dagger}_{i+\delta}c_i+\sum_i(\epsilon_i+\gamma_i)n_i+H_{\text{phon}}\,, \qquad (3.1)$$

with

$$\gamma_i\equiv\sum_s \lambda_s(b^{\dagger}_{is}+b_{is})\,, \qquad (3.2)$$

where sites i and $i+\delta$ are nearest neighbors, ϵ_i is a random-site energy, and $b^{\dagger}_{is}$ creates a phonon of frequency ω_s on site i. We neglect correlation of phonon amplitudes on different sites. This assumption of local phonon modes vastly simplifies the numerical calculations by making the phonon contribution to the electron self-energy site diagonal, thereby precluding the necessity of performing momentum summations over the Brillouin zone. In addition this assumption, though crude, is physically reasonable for systems at temperatures greater than the Debye temperature (a condition which will be assumed in Sec. V), since phonons of all wavelengths will be thermally excited and the phonon correlation function will therefore be short ranged. Furthermore, long-wavelength phonons are of little importance in a system with a short electronic mean free path.[11]

The Fermi level is taken to be at the center of the band. This assumption and the choice of site energy distribution minimizes the structure in the average density of states. We consider two different distributions for the random-site energies. For numerical studies, the Anderson model[25] with a flat distribution between $\pm\frac{1}{2}V$ is convenient. For analytical purposes the Lloyd model, which has a Lorentzian distribution centered on zero, is preferred.

We shall evaluate the conductivity using the Kubo formula which relates the conductivity to the current-current correlation function[28]:

$$\sigma(0)=\lim_{\omega\to 0}\left[-\operatorname{Im}\Pi(\omega+i\delta)/\omega\right]. \qquad (3.3)$$

The retarded response function $\Pi(\omega+i\delta)$ is obtained by analytic continuation from the Matsubara function,[28]

$$\Pi(i\omega)=\frac{-1}{d\Omega}\int_0^{\beta} d\tau\, e^{i\omega\tau}\langle T_\tau\vec{J}(\tau)\cdot\vec{J}(0)\rangle\,, \qquad (3.4)$$

where d is the dimensionality, Ω is the volume of the system, and β is the inverse temperature, $1/k_BT$. The current operator for the Hamiltonian of Eq. (3.1) is

$$\vec{J}=\frac{iet}{\hbar}\sum_{i\delta}\vec{\delta}\,c^{\dagger}_{i+\delta}c_i\,, \qquad (3.5)$$

where $-e$ is the electronic charge. Equations (3.3)–(3.5) may be combined using standard Green's-function techniques to obtain the following exact expression for the dc conductivity (in the absence of phonons):

$$\sigma(0)=\frac{e^2t^2}{d\Omega\hbar}\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi}\left(-\frac{dn_F}{d\epsilon}\right)\sum_{ij}\sum_{\delta\delta'}(-\vec{\delta}\cdot\vec{\delta}')$$
$$\times\langle A_{i,j+\delta'}(\epsilon)A_{j,i+\delta}(\epsilon)\rangle\,, \tag{3.6}$$

where $A_{ij}(\epsilon)=-2\,\mathrm{Im}\,G_{ij}(\epsilon+i\delta)$ is the ij component of the spectral density for the electronic Green's function, $G_{ij}(\epsilon+i\delta)$, $n_F(\epsilon)$ is the Fermi function, and the angular brackets denote the ensemble average over the random-site energies.

In order to evaluate the conductivity in the dirty limit we have chosen to work within the real-space representation rather than the usual momentum-space representation so that the random-site energies are diagonal and the kinetic energy is treated as a perturbation. In the limit of short mean free path the lattice sums in Eq. (3.6) may be conveniently truncated to include only a small cluster of sites. Unfortunately, it is *not* possible to evaluate the ensemble average of the spectral densities required in Eq. (3.6) by simply considering a small cluster because this would never produce Anderson localization. Close to localization the individual random spectral densities develop strong correlated fluctuations which act to suppress the conductivity. This information is lost in any cluster expansion. To date no qualitatively accurate methods for handling this problem have been developed, although progress has recently been made using renormalization-group schemes.[29-32] If one restricts hopping to paths containing no closed loops it turns out that the problem simplifies considerably. We have therefore followed the lead of Abou-Chacra, *et al.*[33] who found that it is possible to study Anderson localization on the Cayley tree (Bethe lattice). A Cayley tree is a lattice (see Fig. 1) containing no closed loops and having a fixed connectivity, K (i.e., each site has $K+1$ neighbors). As Abou-Chacra, *et al.* have shown it is possible to obtain fairly easily and accurately by numerical means the random distribution of spectral functions required in Eq. (3.6), even when the disorder is so large as to produce localization. There remains a problem, however, in that the vector directions required in Eq. (3.6) are ill-defined on the Cayley tree. It is possible (as will be shown) to construct a natural extension of Eq. (3.6) for the Cayley tree.

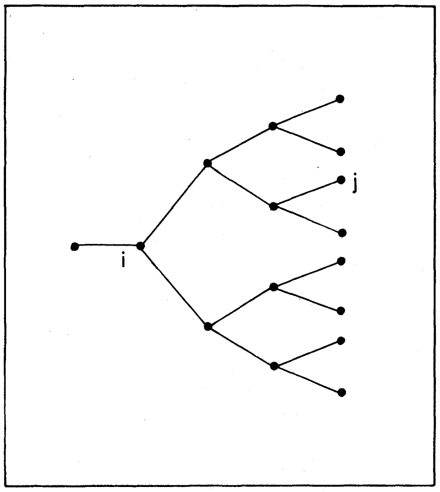

FIG. 1. Cayley tree of connectivity $K=2$. Note that only one path connects sites i and j.

The conductivity (without phonons) which we calculate (see Fig. 2) has the correct limiting properties in that it diverges for zero disorder and vanishes suddenly when Anderson localization occurs. The critical value of disorder at which the conductivity vanishes is in excellent agreement with the value obtained by Abou-Chacra, *et al.* for critical localization. It should be emphasized that in the absence of phonons the conductivity is essentially temperature independent. This results from the constancy of the density of states near the Fermi level which has been built into the model. We do not consider the situation in which the Fermi level lies below the mobility edge and the finite energy width of the factor $(-dn_F/d\epsilon)$ gives rise to activated conduction.

We now turn to a discussion of the details of the calculation. To illustrate the calculation of the spectral density A_{ij} we consider first a system without phonons. Rather than calculating the spectral density directly, it is convenient to consider

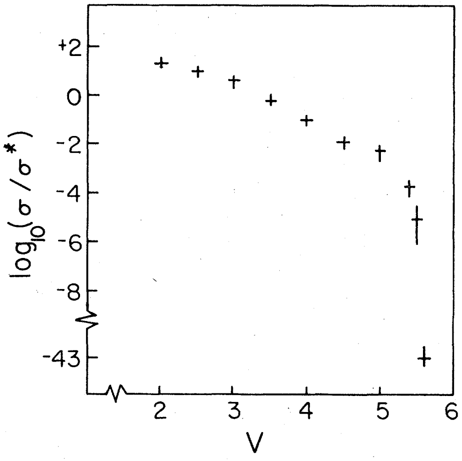

FIG. 2. Conductivity of a Cayley tree of connectivity $K=2$ as a function of disorder (V). Note the broken scales.

$\sigma_i(\epsilon)$, which is the hopping self-energy for all forward-going paths from site i. For a Cayley tree of connectivity K, σ_i satisfies[33]

$$\sigma_i(\epsilon)=\sum_{k=1}^{K}\frac{t^2}{\epsilon-\epsilon_{i+k}-\sigma_{i+k}(\epsilon)}\,. \tag{3.7}$$

Given the probability distribution for the random-site energies ϵ_j, Eq. (3.7) constitutes a recursion relation for the probability distribution of the random self-energies σ_i. Note that σ_i in Eq. (3.7) is independent of ϵ_i, the site energy at the same site. Hence the random variables σ_i and ϵ_i are uncorrelated. We chose to solve Eq. (3.7) for the probability distribution of the hopping self-energy with a numerical Monte Carlo scheme (which will be described in Sec. VII) somewhat different from that of Abou-Chacra *et al.*[33]

Knowing the self-energies σ_i, one may calculate the required spectral functions from

$$A_{ij}(\epsilon)=-2\,\mathrm{Im}G_{ij}(\epsilon)\,, \tag{3.8}$$

$$G_{ij}(\epsilon)=G_{ij-1}(\epsilon)\frac{t}{\epsilon-\epsilon_j-\sigma_j(\epsilon)}\,, \tag{3.9}$$

and

$$G_{ii}(\epsilon)=\frac{1}{\epsilon-\epsilon_i-\sigma_i^t(\epsilon)}\,, \tag{3.10}$$

where σ_i^t in Eq. (3.10), in contrast to σ_i, describes hops on *all* paths from site i. For example, if there is no disorder, i.e., $\epsilon_i=0$ for all i, one readily finds that

$$\sigma_i(\epsilon)=[\epsilon-(\epsilon^2-4Kt^2)^{1/2}]/2\,, \tag{3.11}$$

with the branch of the root being chosen so that σ_i lies in the lower half-complex plane. The local spectral density is given by

$$A_{ii}(\epsilon)=\frac{\theta(4Kt^2-\epsilon^2)(K+1)(4Kt^2-\epsilon^2)^{1/2}}{[\frac{1}{2}(K-1)]^2\epsilon^2+[\frac{1}{2}(K+1)]^2(4Kt^2-\epsilon^2)}\,. \tag{3.12}$$

We shall henceforth express all results in units where $4Kt^2=1$ so that the unperturbed tight-binding band edges are at ±1.

IV. EVALUATION OF THE KUBO FORMULA

Having established a procedure for calculation of the electron Green's function we turn now to the evaluation of the correlation function related to the conductivity. This is the Kubo formula of Eq. (3.6).

One expects for strong disorder, where the mean free path is short, that the position space summation [over j for fixed i, for example, in Eq. (3.6)] will converge rapidly. The lowest-order term in the sum is for i and j being nearest neighbors. The corresponding two-site contribution to the conductivity, σ_0, is for a cubic lattice

$$\sigma_0(0)=\frac{ze^2t^2\delta^2N}{d\Omega\hbar}\times\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi}\left(-\frac{dn_F}{d\epsilon}\right)\langle A_{ii}(\epsilon)A_{jj}(\epsilon)-A_{ij}(\epsilon)A_{ji}(\epsilon)\rangle\,, \tag{4.1}$$

where $N/\Omega=\delta^{-3}$ is the site density and z is the coordination number. Note that as a result of the symmetry of the ensemble-averaged system, Eq. (4.1) is independent of the initial site i, and all z of the nearest-neighbor sites j are equivalent. It is extremely important to note that even though Eq. (4.1) explicitly involves only two sites, the spectral functions depend on the random-site energies on *all* the sites. The ensemble average is therefore nontrivial to perform even for this lowest-order term.

The full expression for the conductivity may be written as

$$\sigma(0)=\sigma_0(0)\Lambda(0)\,, \tag{4.2}$$

where $\Lambda(0)$ is a vertex correction that represents hops to sites outside the initial pair i and j. The vertex function diverges for vanishing disorder and zero temperature because the mean free path is infinite. For large disorder and/or high temperature the mean free path is short and $\Lambda(0)$ becomes of order unity, since the two-site contribution dominates the summation in Eq. (3.6). The form of Eq. (4.2) is convenient because Λ turns out to be a smooth function of disorder and temperature. We note in particular that the complex information about Anderson localization is fully contained in the two-site term, $\sigma_0(0)$ of Eq. (4.2). This is in contrast to the wave-vector representation of the Kubo formula where this information is entirely contained in the vertex function. Using the real-space representation means that the essential physics we wish to discuss is contained in the two-site conductivity term. This is useful because it turns out to be fairly easy to evaluate numerically and yields results with relatively little statistical noise. In addition, there is a problem in evaluating the Kubo formula on a Cayley tree due to the lack of well-defined directions. This problem, however, affects only the vertex function and not $\sigma_0(0)$, which is the object of primary importance. It will be shown below that is it possible to make a reasonable estimate of the true vertex function for the real lattice by considering a natural extension of this function to the Cayley tree.

The lack of well-defined directions is not a problem in one dimension where the actual lattice and the Cayley tree of connectivity $K=1$ are identical. Let us therefore begin by considering the conductivity in one dimension. It is convenient to define a quantity S by

$$S \equiv \frac{t^2}{Nz\delta^2} \sum_{ij\delta\delta'} (-\vec{\delta}\cdot\vec{\delta}')\langle A_{i,j+\delta'}A_{j,i+\delta}\rangle , \tag{4.3}$$

where $\pm\vec{\delta}$ are nearest-neighbor lattice vectors. Performing the lattice sums, relabeling dummy indices, and using the symmetry of the spectral density $A_{ij}=A_{ji}$, one can express Eq. (4.3) as

$$S = a_1 + 2\sum_{n=2}^{\infty} a_n , \tag{4.4}$$

where

$$a_n \equiv t^2\langle A_{i,i+n-1}A_{i+1,i+n} - A_{i,i+n}A_{i+1,i+n-1}\rangle . \tag{4.5}$$

Again, because of the translational symmetry, the ensemble-averaged quantity a_n depends only on n.

In going from Eq. (4.3) to Eq. (4.4) we have also used the fact that in one dimension $\vec{\delta}\cdot\vec{\delta}'=\pm\delta^2$, since $\vec{\delta}$ and $\vec{\delta}'$ are either parallel or antiparallel. If one now considers the chain of sites connecting site i and site j ($j=i+n$) on the Cayley tree of Fig. 1, one sees that this resembles the one-dimensional lattice, except that $|\vec{\delta}\cdot\vec{\delta}'|/\delta^2$ may differ from unity. The two-site contribution, though, is still given by Eq. (4.5) with $n=1$. This is because $\vec{\delta}'=\pm\vec{\delta}$ in those terms in Eq. (4.3) which contribute to a_1. For terms a_n that involve longer chains ($n>2$), we have arbitrarily taken $\vec{\delta}\cdot\vec{\delta}'$ to be $\pm\frac{1}{2}\delta^2$, using the general "forward" and "backward" directions of the Cayley tree to determine the sign. Noting that the Cayley tree has zK^{n-1} chains of length n emanating from a given site suggests the following form as a natural extension of S to the Cayley tree:

$$S = \sum_{n=1}^{\infty} K^{n-1}a_n , \tag{4.6}$$

where a_n is still given by Eq. (4.5). It is convenient to use Eq. (3.9) and Eq. (3.10) to express a_n as

$$a_n(\epsilon) = 4\left\langle |G_{ii}(\epsilon)|^2(\mathrm{Im}\tilde{\sigma}_i)(\mathrm{Im}\sigma_{i+n}) \prod_{k=1}^{n} \frac{t^2}{|\epsilon-\epsilon_{i+k}-\sigma_{i+k}|^2}\right\rangle . \tag{4.7}$$

Referring to the chain of sites between i and j in Fig. 1, σ_k is the self-energy for hops from a site k (in the chain) in all directions except backwards along the chain (toward site i), and $\tilde{\sigma}_k$ represents hops in all directions except forward along the chain (toward site j). By combining Eq. (3.6) with Eqs. (4.3)–(4.7) and letting the number of nearest neighbors z be six while allowing the connectivity K to be different from $z-1$, one obtains the following Cayley-tree approximation to the conductivity of a three-dimensional simple-cubic system:

$$\sigma(0) = \frac{e^2}{\hbar\delta\pi}\int_{-\infty}^{\infty} d\epsilon \left(-\frac{dn_F}{d\epsilon}\right)\sum_{n=1}^{\infty} K^{n-1}a_n(\epsilon) . \tag{4.8}$$

The integration over energy ϵ in Eq. (4.8) introduces a thermal broadening of width k_BT around the Fermi level. As mentioned earlier, the model has been intentionally chosen so that the density of states and the mobility are essentially energy independent in the center of the band which is the location of the Fermi level. We therefore replace Eq. (4.8) by

$$\sigma(0) = \frac{e^2}{\hbar\delta\pi}\sum_{n=1}^{\infty} K^{n-1}a_n(0) . \tag{4.9}$$

The two-site contribution is thus

$$\sigma_0(0) = (e^2/\hbar\delta\pi)a_1(0) , \tag{4.10}$$

and the vertex function is

$$\Lambda(0) = \sum_{n=1}^{\infty} K^{n-1}\frac{a_n(0)}{a_1(0)} . \tag{4.11}$$

We again emphasize that the phrase "two-site" does not refer to a cluster calculation restricted to two sites only. The ensemble averages in Eqs. (4.10) and (4.11) involve the entire lattice.

The approximations used to circumvent the difficulties connected with the lack of well-defined directions on the Cayley tree are admittedly somewhat arbitrary. However, the vertex function calculated in Eq. (4.11) has the correct limiting features in that it diverges for zero disorder and becomes of order unity for large disorder. Furthermore, in the high-disorder regime the two-site term of Eq. (4.10), which is unaffected by these approximations, is the major contributor to the conductivity. These considerations suggest that we have a method of calculating the conductivity which is at least qualitatively correct over the entire range of disorder from very weak to very strong (including the regime of Anderson localization).

V. ELECTRON-PHONON INTERACTION

We consider first the effect of the electron-phonon interaction in perturbation theory. The lowest-order phonon self-energy for site i due to the phonons at site i is given in the Matsubara notation by

$$\Sigma_i(i\omega) = -\sum_{s} |\lambda_s|^2\beta^{-1}\sum_{i\Omega} D_{is}(i\Omega)G_{ii}(i\omega+i\Omega) , \tag{5.1}$$

where $D_{is}(i\Omega)$ is the phonon propagator. This self-energy simply adds to the hopping self-energy in Eqs. (3.9) and (3.10), and Eq. (3.7) becomes

$$\sigma_i(\epsilon)=\sum_{k=1}^{K}\frac{t^2}{\epsilon-\epsilon_{i+k}-\sigma_{i+k}(\epsilon)-\Sigma_{i+k}(\epsilon)}\,. \tag{5.2}$$

Recall that σ_i is the self-energy for forward-going hops and thus in the absence of phonons depends only on those site energies forward of site i. The phonon self-energy complicates the situation by introducing a dependence on all the site energies. It turns out, however, that this complication can be ignored without significant numerical error in the final results.

In order to calculate the retarded electron-phonon self-energy, the Matsubara sum in Eq. (5.1) must be evaluated. One finds that

$$\Sigma_i(\epsilon+i\delta)=\sum_s|\lambda_s|^2\int_{-\infty}^{\infty}\frac{d\epsilon'}{2\pi}A_{ii}(\epsilon')\left(\frac{n_F(\epsilon')+n_B(\omega_s)}{\epsilon-\epsilon'+\omega_s+i\delta}+\frac{1-n_F(\epsilon')+n_B(\omega_s)}{\epsilon-\epsilon'-\omega_s+i\delta}\right). \tag{5.3}$$

This result simplifies considerably if the temperature is high compared to the Debye temperature, in which case $n_B(\omega_s)\simeq k_BT/\omega_s>n_F(\epsilon')$. This assumption will hereafter be implicit. In particular, the imaginary part of the self-energy simplifies to

$$\mathrm{Im}\Sigma_i(\epsilon+i\delta)=-\frac{k_BT}{2}\int_{-\infty}^{\infty}dx\,g(x)A_{ii}(\epsilon+x)\,, \tag{5.4}$$

where

$$g(x)\equiv\sum_s\frac{|\lambda_s|^2}{\omega_s}[\delta(x-\omega_s)+\delta(x+\omega_s)]\,. \tag{5.5}$$

The dynamics of the electron-phonon interaction enters Eqs. (5.3) and (5.4) as a convolution of the electron spectral density over the phonon frequencies. The adiabatic-phonon approximation amounts to neglecting the energy transfer to the electron, which yields

$$\Sigma_i^{\mathrm{stat}}(\epsilon+i\delta)=k_BT\bar{g}G_{ii}(\epsilon+i\delta)\,, \tag{5.6}$$

and in particular

$$\mathrm{Im}\Sigma_i^{\mathrm{stat}}(\epsilon+i\delta)=-(k_BT/2)\bar{g}A_{ii}(\epsilon)\,, \tag{5.7}$$

where

$$\bar{g}\equiv\int_{-\infty}^{\infty}dx\,g(x)\,. \tag{5.8}$$

It is instructive to compare the results that retain the electron-phonon dynamics [Eqs. (5.3) and (5.4)] with the adiabatic approximation [Eqs. (5.6) and (5.7)]. First we note that in the zero-disorder limit the real part of the self-energy vanishes at the Fermi level (the center of the band) in both cases. If, in the absence of disorder, we neglect density-of-states effects, i.e., take $A_{ii}(\epsilon)$ to be independent of energy in the range $-\hbar\,\omega_{\mathrm{Deb}}<\epsilon<\hbar\,\omega_{\mathrm{Deb}}$, we have from Eqs. (5.4)–(5.7) that the adiabatic- (static-) phonon approximation is exact for $\mathrm{Im}\Sigma_i$ in this limit. Now, as the disorder is increased, structure develops in the spectral density (although not in the ensemble-averaged spectral density). For strong disorder the spectral density consists of a set of sharp peaks separated by regions of nearly zero density. (Indeed, when the disorder is large enough to localize the electrons, the spectral density will consist of a set of delta functions.) In the strong-disorder limit the convolution over phonon frequencies in Eq. (5.4) makes $\mathrm{Im}\Sigma_i(\epsilon)$ nonzero for all ϵ, while the static result is nearly zero almost everywhere. *The static approximation therefore fails in this limit.* This is a key point. It makes absolutely no difference in calculating the ensemble-averaged spectral density, but as we shall see it strongly affects the conductivity (which is the ensemble average of the product of two spectral densities).

As a matter of convenience, the real part of the electron-phonon self-energy will be neglected, since in the large-disorder limit it is much smaller than the fluctuations in the random-site energies. Actually, to perform the frequency integration in Eq. (5.4) would be a numerically difficult problem in the strong-disorder limit. However, by approximating $g(\omega)$ as a Lorentzian

$$g(\omega)=\omega_D\bar{g}/\pi(\omega^2+\omega_D^2) \tag{5.9}$$

of width ω_D, taken to be the Debye energy, the required frequency integral can be easily performed analytically:

$$\mathrm{Im}\Sigma_i(\epsilon+i\delta)=k_BT\bar{g}\,\mathrm{Im}G_{ii}(\epsilon+i\omega_D)\,. \tag{5.10}$$

It is clear from the discussion of the previous sections that $G_{ii}(\epsilon+i\omega_D)$ is easily evaluated by the same methods used to find $G_{ii}(\epsilon+i\delta)$. The approximation leading to Eq. (5.10) may be justified *a posteriori* by the observation that the results are essentially independent of the choice for ω_D (taken in this case to be 0.01 in units of the half-bandwidth).

In summary, we find that the static approximation to the electron-phonon interaction is good for weak disorder, but the fact that the electrons can exchange energy with the phonons becomes crucial for strong disorder. These results were established in perturbation theory. However, if we have only static phonons, we do not have to confine ourselves to perturbation theory. In fact, we can solve the static-phonon problem exactly by simply adding to each site energy ϵ_i an additional energy γ_i whose probability distribution is a Gaussian of width

$$\langle \gamma_i^2 \rangle = k_B T \overline{g} . \tag{5.11}$$

We shall take maximum advantage of this fact by treating the static part of the electron-phonon interaction exactly and by including the dynamic part in lowest-order perturbation theory. The latter is given by the difference

$$\Delta\Sigma_i = \Sigma_i - \Sigma_i^{\text{stat}} . \tag{5.12}$$

As discussed above, this difference tends to zero in the absence of disorder when the static approximation is exact, but becomes important when the disorder is large. The real part of $\Delta\Sigma_i$ was found to be of little importance in the numerical calculation and so was set equal to zero.

In addition to phonon self-energy corrections there are phonon vertex corrections which also affect the conductivity. Since we are treating the static-phonon effects exactly these vertex corrections are automatically included. We neglect any dynamic contribution to the vertex function.

Finally, we note that the electron-phonon coupling $\overline{g}$ defined by Eqs. (5.5) and (5.8) is related to McMillan's parameter[34] λ via

$$\overline{g} \simeq \lambda W , \tag{5.13}$$

where W is the bandwidth. We arbitrarily take $\lambda = 0.25$ and $W = 5$ eV so that $\overline{g} = 1.25$ eV. This choice is consistent with the deformation-potential estimate of $\overline{g}$ made by Chen *et al.*[18]

In summary, there are two effects of the electron-phonon interaction within the approximation used here. The first is an increase in the static disorder due to the presence of an additional random-site energy γ_i on each site. The second is an increase in the hopping self-energy due to an imaginary self-energy $i\,\text{Im}\Delta\Sigma_i$ produced by the phonon dynamics. These two corrections enter the expression for the conductivity [Eq. (4.7)] and also enter the right-hand side of the recursion relation [Eq. (3.7)] that determines the probability distribution of the hopping self-energies σ_i.

VI. ANALYTIC RESULTS

A. Neglect of correlations

Within certain approximations, it is possible to obtain analytic results showing the role of phonon dynamics in the conductivity of disordered systems. While the approximations involved are necessarily rather extreme, it is useful to consider these results in order to gain greater insight into the essential physics of the problem before going on to discuss the details of the full numerical calculations.

Some basic conclusions may be drawn directly from the fact that the conductivity [Eq. (3.6)] is related to a configurational average of a product of spectral functions of the form

$$f = \langle A_{ij} A_{kl} \rangle , \tag{6.1}$$

rather than to a product of average spectral functions of the form

$$h = \langle A_{ij} \rangle \langle A_{kl} \rangle . \tag{6.2}$$

The latter quantity would determine the conductivity if correlations between the two spectral functions were neglected. We begin with a consideration of this approximation. Equation (6.2) may be exactly evaluated within the Lloyd model[35] in which the random-site energies have a Lorentzian probability distribution

$$P(\epsilon_i) = \gamma / [\pi(\epsilon^2 + \gamma^2)] . \tag{6.3}$$

The Lloyd model has the interesting property that the *average* effect of the random potential is precisely equivalent to the effect of a uniform coherent (optical) potential

$$V_c = -i\gamma \tag{6.4}$$

on each site. One obtains

$$\langle A_{ij}(\epsilon) \rangle = -2\,\text{Im} g_{ij}(\epsilon + i\gamma) , \tag{6.5}$$

where g_{ij} is the Green's function in the absence of disorder, a quantity which is easily calculable for any lattice. Hence if correlations are ignored, the conductivity may be evaluated exactly and is found for small disorder to be simply proportional to the mean free time

$$\sigma(0) = P/\gamma , \tag{6.6}$$

where P is a constant depending on the particular lattice. For very large disorder, the conductivity is proportional to the square of the average density of states at the Fermi level:

$$\sigma(0) = P'/\gamma^2 . \tag{6.7}$$

Thus the conductivity diverges for zero disorder and goes continuously to zero with increasing disorder.

One must now ask how phonons affect the situation. Equation (5.4) gives the lowest-order phonon self-energy. This is a random quantity since it involves the spectral function $A_{ii}(\epsilon)$, which in turn depends on the random-site energies. However, the phonon self-energy fluctuates much less strongly than the spectral function since it involves an average of the spectral function over different frequencies. Indeed, in the extreme case of white-noise phonons[36] one has $g(x)=\overline{g}$ in Eqs. (5.3) and (5.4), and

$$\Sigma_{\text{ph}}=-i\pi k_B T\overline{g} \tag{6.8}$$

is the *exact* phonon self-energy, which does not fluctuate at all. For the purpose of making analytic calculations, we therefore assume that the phonon self-energy may be replaced by its average value

$$\Sigma_{\text{ph}}=-i\xi , \tag{6.9}$$

where ξ increases with temperature. In the presence of phonons Eq. (6.5) becomes

$$\langle A_{ij}(\epsilon)\rangle=-2\,\text{Im}g_{ij}(\epsilon+i\gamma+i\xi) . \tag{6.10}$$

Hence the effect of phonons is exactly the same as that of the static random-site-energy disorder (i.e., the static-phonon approximation is exact), and for small disorder the conductivity becomes

$$\sigma(0)=P/(\gamma+\xi) , \tag{6.11}$$

in accordance with Mattheissen's rule [Eq. (2.3)]. For large disorder the conductivity is

$$\sigma(0)=P'/(\gamma+\xi)^2 . \tag{6.12}$$

For all values of disorder the phonons act to decrease the conductivity. Equation (6.11) satisfies Eq. (2.4) as an equality. Equation (6.12) on the other hand satisfies only the inequality.

If correlations between spectral functions are neglected one can explicitly evaluate the Cayley-tree approximation to the conductivity given by Eq. (4.9):

$$\sigma(0)=\frac{e^2}{\hbar\delta\pi}\,\frac{\Delta(\gamma+\xi+\Delta)^4}{(\gamma+\xi)[(\gamma+\xi+\Delta)^2+t^2]^2} , \tag{6.13}$$

where

$$-i\Delta=(-i/2)\{[4Kt^2+(\gamma+\xi)^2]^{1/2}-(\gamma+\xi)\} \tag{6.14}$$

is the ensemble-averaged forward-hopping self-energy. Equation (6.14) conforms to the large and small disorder limits given above, and the conductivity is a monotomically decreasing function of both disorder (γ) and temperature (ξ).

One is thus led to the conclusion that there is an intimate connection between the failure of the Boltzmann formalism and the neglect of correlations between the spectral functions in the conductivity. The approximation made in Eq. (6.2) is reasonable for weak disorder (where the Boltzmann theory is valid), but in the presence of strong disorder it is essential to retain the correlations between the spectral functions as in Eq. (6.1). These correlations are the key to the negative TCR (in our model). Their retention in an analytic scheme is a difficult task, but by making certain approximations one can at least illustrate the effect. This is the scope of the next subsection.

B. Inclusion of correlations

In Sec. IV the conductivity was found to have the form

$$\sigma(0)=(e^2/\hbar\delta\pi)a_1(0)\Lambda(0) , \tag{6.15}$$

where

$$a_1(0)\equiv t^2\langle A_{ii}A_{jj}-A_{ij}A_{ji}\rangle , \tag{6.16}$$

and sites i and j are nearest neighbors. This form is convenient because in order to proceed analytically it is necessary to make the major approximation of considering only the random-site energies ϵ_i and ϵ_j explicitly and of treating the disorder on other sites only in an average sense, by introducing the optical potential of Eq. (6.4). This simplification severely underestimates the complex fluctuations in the spectral functions; however, this is partially compensated by the fact that Eq. (6.9) overestimates the dynamic-phonon effect. The qualitative effect of correlations will still be present in Eq. (6.16).

As noted earlier, the required Green's functions are particularly easy to evaluate if i and j are considered to be adjacent sites embedded in a Cayley tree. For example, one has

$$G_{ii}(\epsilon)=\frac{(\epsilon+i\xi-\epsilon_j-\Sigma)}{(\epsilon+i\xi-\epsilon_i-\Sigma)(\epsilon+i\xi-\epsilon_j-\Sigma)-t^2} , \tag{6.17}$$

where Σ is the (ensemble-averaged) self-energy for hops to sites other than i and j. Note that G_{ii} depends on both ϵ_i and ϵ_j so that fluctuations in G_{ii} and G_{jj} are correlated. This tends to reduce the conductivity [through the factor $a_1(0)$ in Eq. (6.15)] and in a complete theory would ultimately lead to Anderson localization ($a_1=0$). In the present approximation Eq. (6.15) becomes

$$a_1(0)=\left\langle\frac{4t^2\eta^2}{|(\epsilon_i-i\eta)(\epsilon_j-i\eta)-t^2|^2}\right\rangle , \tag{6.18}$$

where $\eta\equiv\xi+\Delta$. Since the phonon self-energy $-i\xi$ scales with temperatures and since $d\eta/d\xi>0$, one sees that the TCR is related to $(-d\ln a_1/d\eta)$ (delaying for the moment a discussion of the temperature dependence of the vertex function). The average over ϵ_i and ϵ_j in Eq. (6.18) can be performed analytically in the Lloyd model with the result

$$a_1(0)=\frac{4t^2\eta}{\Gamma^2-\gamma^2}\left(\frac{\gamma+\eta}{(\gamma+\eta)^2+t^2}-\frac{\gamma}{\Gamma}\,\frac{\Gamma+\eta}{(\Gamma+\eta)(\gamma+\eta)+t^2}\right) , \tag{6.19}$$

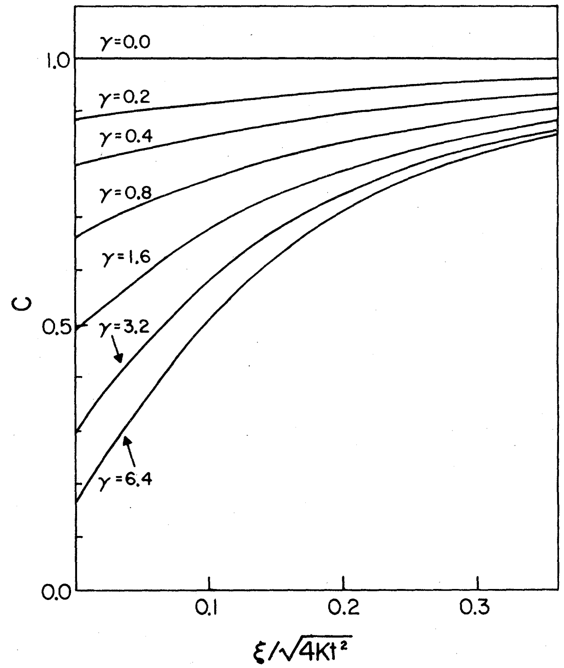

FIG. 3. Correlation factor C of Eq. (6.22) as a function of $\xi/(4Kt^2)^{1/2}$ for different amounts of disorder, γ.

where

$$\Gamma^2 \equiv \eta^2 + t^2 . \tag{6.20}$$

It is interesting to compare this result, which contains correlations, with the no-correlation (NC) value

$$a_{1\,\mathrm{NC}} = \frac{(\gamma+\eta)^2 t^2}{[(\gamma+\eta)^2 + t^2]} . \tag{6.21}$$

One can define a correlation factor C by

$$a_1 = a_{1\,\mathrm{NC}} C . \tag{6.22}$$

The two terms in Eq. (6.22) each contribute to the TCR. As noted earlier, the static disorder and the phonon self-energy enter a_1 in exactly the same way if correlations are neglected. Hence, $-da_{1\,\mathrm{NC}}/d\xi > 0$, which makes a *positive* contribution to the TCR. The correlation factor C depends on the static and phonon disorders in different ways. Figure 3 shows that C decreases with static disorder (γ) but increases with temperature (ξ). This is true for all values of γ and ξ and produces a *negative* contribution to $-da_1/d\xi$. Except for small K the correlation factor C is well approximated by

$$C \simeq \eta/(\eta^2 + t^2)^{1/2} . \tag{6.23}$$

For small disorder the hopping self-energy Δ (and hence η) is large and $C \simeq 1$. For large disorder η is small and $C \simeq 0$. From Eq. (6.23) one has

$$-\frac{d\ln C}{d\xi} = -\frac{t^2}{\eta(\eta^2+t^2)}\frac{d\eta}{d\xi} < 0 . \tag{6.24}$$

For large disorder the derivative becomes increasingly negative. This is the dynamic-phonon effect we have been seeking. The crossover point at which the negative contribution due to the dynamic effect wins out over the static effect of Eq. (6.21) occurs at roughly $\eta = t$ (more or less independent of the lattice connectivity K). That this is reasonable can be seen from an inspection of Eq. (6.18), which shows that correlations strongly affect a_1 only for $\eta \lesssim t$. From Eq. (6.23) it follows that at the critical resistivity, $C \simeq 1/\sqrt{2}$ in this approximation.

Thus far the effect of phonons on the vertex function Λ has not been included. In the present approximation in which fluctuating site energies are retained only on two sites, it is possible to calculate Λ from Eq. (4.11) analytically. The result is

$$\Lambda(0) = 1 + \left(\frac{\Delta}{\Delta+\xi}\right)\sum_{n=1}^{\infty}\left(\frac{\Delta}{\gamma+\Delta+\xi}\right)^{n-1} , \tag{6.25}$$

$$\Lambda(0) = 1 + \frac{\Delta}{\Delta+\xi}\,\frac{\gamma+\xi+\Delta}{\gamma+\xi} . \tag{6.26}$$

The nth term in Eq. (6.25) is associated with paths terminating n sites away from the central pair of sites i and j. Note that as expected, $\Lambda(0)$ diverges in the limit of vanishing disorder and temperature but becomes of order unity in the limit of strong disorder and/or high temperature. The vertex correction is a monotonically decreasing function of both disorder (γ) and temperature (ξ) and therefore contributes a positive term to the TCR. This is also the case in the full numerical calculations (where all correlations are included), and we attribute this to the fact that the electron mean free path is decreased by both elastic (disorder) and inelastic (phonon) scattering. This positive contribution to the TCR is large for small disorder and dominates over the correlation effects which are weak. For large disorder, correlation effects are strong enough to produce a negative TCR. However, if the phonon self-energy $-i\xi$ is large enough so that $\eta > t$ in Eq. (6.18) correlations are weakened, the density of states is lowered, and the mean free path is shortened. Hence the TCR becomes positive again at very high temperatures. This behavior is illustrated in Fig. 4. As will be shown in the next section, this picture is confirmed by the full numerical calculations.

It is interesting to note that one can anticipate

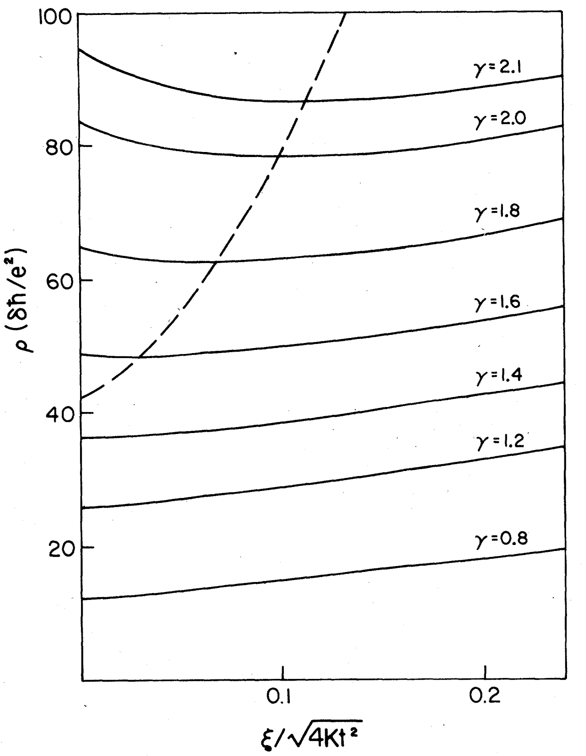

FIG. 4. Resistivity versus temperature $[\xi/(4Kt^2)^{1/2}]$ in a model with two fluctuating site energies (see text). The strength of the disorder, γ, is indicated and the broken line represents the loci of zero TCR. With $|\vec{\delta}|=3$ Å, $\delta\hbar/e^2=123\ \mu\Omega\,\mathrm{cm}$.

several features of the full numerical calculation from Eq. (6.25). Note that at zero temperature ($\xi=0$) the three-site contribution ($n=1$ term in the summation) is equal to unity, which is the same as the two-site contribution. In the numerical calculation (with fluctuating site energies on all sites), it was found that the first M terms each contribute roughly unity to the vertex function while contributions from larger distances quickly dropped to zero. The value of M is a function of disorder and is related to the elastic mean free path. At finite temperatures on the other hand the multisite contributions to the vertex function decreased continuously with distance even at small distances, just as the $n=1$ term of Eq. (6.25) is less than unity at finite temperatures.

The physical picture one obtains from analytic consideration of the Lloyd model may be summarized in the following manner. The *average* effect of the random potential is to introduce a uniform optical potential $V_c=-i\gamma$. Added to this is an imaginary phonon self-energy $-i\xi$. For low disorder (γ small) it is best to work in the plane-wave representation, where V_c represents a decay rate for the plane-wave modes. Increasing the temperature increases $V_c-i\xi$ and hence reduces the mean free time of the electrons. This enhances the resistivity in a manner consistent with Matthiessen's rule.

For a strong disorder, the effect of the potential cannot be treated in an average way, and because of the strong scattering it is preferable to work in the site representation. Due to the strong disorder it is difficult for an electron to diffuse through the lattice and hence the hopping self-energy for a given site is typically small. Adding phonon dynamics increases the imaginary self-energy. This represents an enhanced ability of the electrons to diffuse away into the rest of the lattice.

The analytic simplicity of the Lloyd model has allowed illustration of several key technical considerations which must be carried along with the physical picture. First, for weak disorder Matthiessen's rule was explicitly verified. Second, it was shown that the Boltzmann picture which produces Matthiessen's rule follows from a neglect of the correlation between the random spectral functions entering the Kubo formula. Hence it must be these correlations which lead to the resistivity anomaly. These considerations show that there are two competing phonon contributions to the TCR. Static-phonon effects decrease the mean free path and for strong coupling decrease the density of states at the Fermi level. On the other hand the phonon dynamics thwarts the correlation effects which would otherwise decrease the conductivity. The former dominates for small disorder, the latter for large.

VII. NUMERICAL RESULTS

In our numerical calculations we used a Monte Carlo technique somewhat different from that of Abou-Chacra *et al.*[33] to solve Eq. (5.2) for the probability distribution of the random hopping self-energies, $\sigma_i(\epsilon)$ and $\sigma_i(\epsilon+i\omega_D)$ needed to evaluate the conductivity in the presence of phonons. The procedure is as follows. Starting with two initial ensembles of 4000 (complex) self-energies $[\sigma_i(0)]$ and $[\sigma_i(i\omega_D)]$, K elements are picked at random from one ensemble along with the K *corresponding* elements from the other ensemble. Next, K random-site energies are generated using a flat probability distribution between $\pm\frac{1}{2}V$. These parameters are used in Eqs. (5.7), (5.10), and (5.12) to calculate K values of $\Delta\Sigma_i$, the dynamic part of the electron-phonon interaction. The next step is to generate K values of γ_i, the static part of the electron-phonon interaction, using a Gaussian distribution of width $\bar{g}k_BT$ [see Eq. (5.11)].

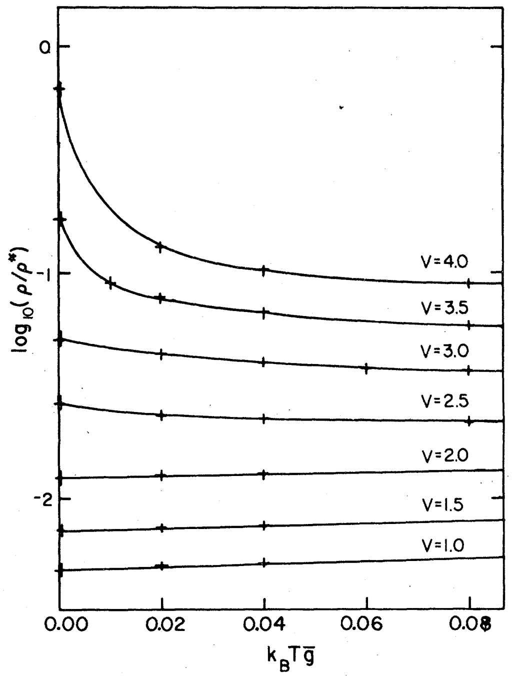

FIG. 5. Resistivity as a function of $\bar{g}k_BT$ (electron-phonon coupling times temperature) for various amounts of disorder (V) calculated in the two-site approximation (see text). Energy units are chosen so that $W/2=1$, W being the bandwidth.

Since it is rather expensive to generate Gaussian random numbers, we found it advantageous to create a field of 10^4 such numbers and sample this field at random in order to assign values to γ_i (in a typical ensemble average of the conductivity, 10^6–10^7 values were required). One now has all the parameters needed to calculate one new value each of $\sigma_i(0)$ and $\sigma_i(i\omega_D)$ from their respective recursion relations. The first elements of the two initial ensembles are replaced with these new values. The process is then repeated to generate replacements for the second elements, and so on until all 4000 elements have each been replaced up to 100 times.

The above procedure, which must be repeated for each temperature and value of disorder, converges rapidly from almost any initial ensemble except in the region of critical localization where care must be exercized. As mentioned in Sec. V, the electron-phonon interaction causes σ_i to depend on site energies over the entire lattice rather than just those site energies for sites forward of i (as is assumed in the recursion relations). However, the dependence is very weak, and numerical tests show that this complication can be safely ignored as was done in the calculations reported here.

Having obtained ensembles representing the probability distributions of $\sigma_i(0)$ and $\sigma_i(i\omega_D)$ for particular values of the temperature and disorder, we are now ready to calculate the ensemble-averaged conductivity. The number of terms N retained in the summation in Eq. (4.9) and the number of different site energy configurations M used in evaluating the ensemble average varied with disorder. For weak disorder ($V=2$), $N=100$ and $M=5000$ were used, while close to the localization threshold ($V=5$), $N=20$ and $M=15\,000$ were used. Each configuration was defined by a set of $N+1$ site energies and hopping self-energies generated from the appropriate probability distributions (ensembles) and the recursion relation Eq. (5.2).

The results of the numerical calculations are shown in the figures. Figure 2 shows the conductivity as a function of disorder at zero temperature. The critical value of disorder, $V^*=5.5\,(4Kt^2)^{1/2}$, is in excellent agreement with the value obtained by Abou-Chacra *et al.*[33] On the other hand, the value of the critical conductivity is roughly two orders of magnitude smaller than Mott's minimum metallic conductivity ($\simeq 0.1\, e^2/\hbar\delta$). We believe this to be an artifact of the Cayley tree, which has an ill-defined dimensionality, and we speculate that a calculation on a real three-dimensional lattice should produce a value of the minimum metallic conductivity in better agreement with Mott's estimates. It should be noted that the strength of disorder necessary to induce Anderson localization in a real lattice[37] seems to be considerably smaller than that required on a Cayley tree.

The temperature-dependent resistivity of Fig. 5 was calculated using the two-site approximation to the Kubo formula. One sees that for weak disorder, there is a small positive TCR, but as the disorder increases the TCR changes sign and becomes increasingly negative. The resistivity in Fig. 6 is based on the full evaluation of the Kubo formula and shows similar behavior although the numerical noise is considerably worse.

There is a remarkable qualitative similarity between Fig. 6 and the crude analytical results of Fig. 4. In particular, one observes in both figures that for strong disorder the TCR changes sign and becomes positive at high temperatures. As discussed in Sec. VI, this is a reflection of the two competing aspects of the electron-phonon interaction. It follows that a Mooij plot of the TCR versus resistivity is temperature dependent, i.e., a material that has a negative TCR at low temperatures could have a positive TCR at high temperatures, with the resistivity being nearly unchanged.

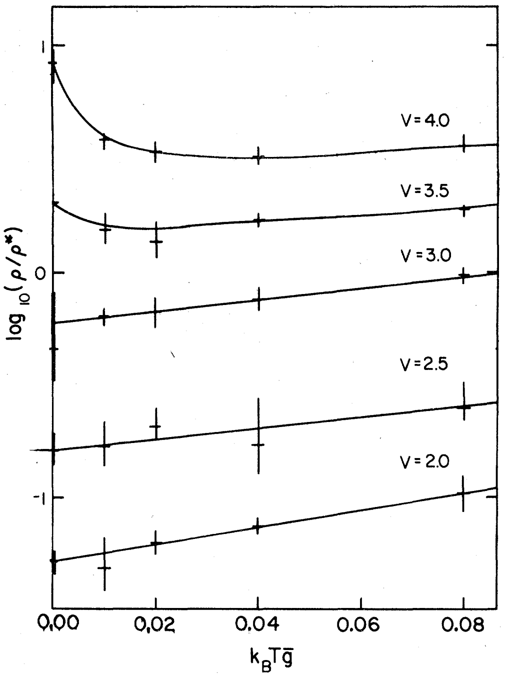

FIG. 6. Resistivity as a function of $\bar{g}k_BT$ (electron-phonon coupling times temperature) for various amounts of disorder (V). Energy units are chosen so that $W/2=1$, W being the bandwidth.

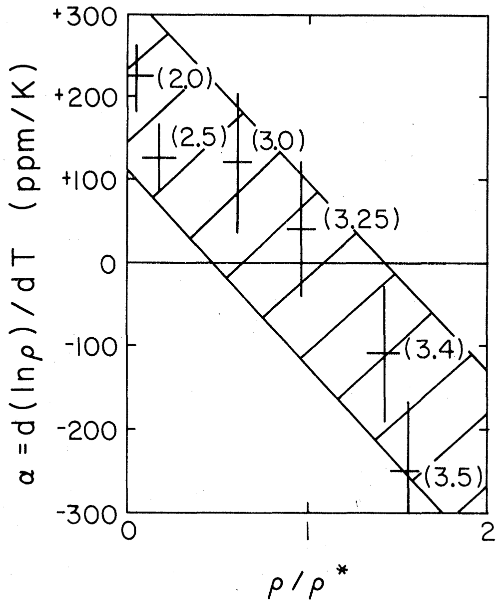

FIG. 7. Temperature coefficient of resistivity (TCR), α as a function of reduced resistivity ρ/ρ^*. The numbers in parentheses indicate the value of V (disorder). The experimental points plotted by Mooij (Ref. 1) fall within the hatched area. From the Mooij plot $\rho^* \simeq 150$ $\mu\Omega$ cm, whereas in our model calculation $\rho^* \simeq 750$ $\mu\Omega$ cm.

This behavior has been observed in some materials.[2]

Figure 7 shows a Mooij plot generated from the results displayed in Fig. 6. All points are for room temperature ($\bar{g}k_BT = 0.005$ in units of $W^2/4$, see Sec. V). Except for an overall scale factor in the resisitivity the results are in qualitative agreement with the observed Mooij correlation. Our Cayley-tree calculation[38] estimates $\rho^* \simeq 750$ $\mu\Omega$ cm for a simple cubic lattice, while experimentally $\rho^* \simeq 150$ $\mu\Omega$ cm.

VIII. SUMMARY AND DISCUSSION

We have presented a theory of transport in metal alloys which focuses on those model-independent features of the electron-phonon interaction which appear in the limit of strong disorder. It was found that the breakdown of the adiabatic-phonon approximation produces a direct correlation between the resistivity and its temperature coefficient which is in qualitative agreement with the Mooij correlation. This effect is quite universal and should generally be present, although in specific cases it may not dominate over the model-dependent mechanisms previously proposed.[6-22]

Some comments need to be made concerning the Cayley-tree approximation. We have already remarked that the conductivity at zero temperature (Fig. 2) exhibits a maximum metallic resistivity much larger than Mott's estimates. Imry[39] has also pointed out that the sharp drop in resistivity of the Cayley tree when localization occurs is inconsistent with the predictions of recent scaling theories[30] of localization in three dimensions. Nevertheless, we do not feel that the Cayley-tree approximation compromises the validity of our central physical idea because fluctuations in the spectral density leading to the inequality

$$\langle A_{ij}A_{kl}\rangle \ll \langle A_{ij}\rangle\langle A_{kl}\rangle \qquad (8.1)$$

certainly occur on real lattices, though they are conveniently calculable only on the Cayley tree.

Calculations on real lattices will also be necessary in order to discuss the resistivity saturation observed in $A15$ compounds[4,5] which cannot be explained by our present results. Clearly, our model of a single tight-binding band with intentionally minimized structure in the density of states is too simple to describe the $A15$'s adequately.

In summary our main purpose in this and a previous paper[23] has been to introduce the new physical idea that phonon-assisted mobility can occur in disordered systems, even in the regime of extended states, and to illustrate the effect qualitatively with a simple model calculation. Clearly, further work is required to make the present model more realistic and to study the relevance of this effect to other transport anomalies.

ACKNOWLEDGMENTS

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APPENDIX

In this Appendix we wish to comment on a recent paper by Imry[39] which applies a scaling theory of localization[30] to the problem of the Mooij correlation. The basic result of this theory is that the conductivity (in the absence of phonons) has the form

$$\sigma = A g_c (e^2/\hbar L_\Omega)\,, \qquad \text{(A1)}$$

where A is a constant of order unity, g_c is a critical dimensionless conductance of order unity, and L_Ω is the length scale at which the conductivity becomes Ohmic. L_Ω increases with disorder and goes to infinity at critical localization. Following Thouless,[40] Imry argues that at finite temperatures the relevant length scale is $L = \min(L_\Omega, l_{\text{ph}})$, where l_{ph} is the inelastic mean free path (due to phonon scattering). For $l_{\text{ph}} < L_\Omega$ the relevant length scale decreases with temperature, thus increasing the conductivity. Highly disordered samples are therefore predicted to exhibit a negative TCR above some temperature T^* whose value depends on disorder. At some higher temperature l_{ph} becomes on the order of a microscopic length, the scaling theory breaks down, and the conductivity presumably starts to decrease again.

Although there is some controversy regarding the validity of the scaling theory, especially for two-dimensional systems,[29] it is interesting to make contact with the present work. To this end we note that Imry's argument may be translated from the language of length scales to time scales. For large disorder the imaginary part of the hopping self-energy for a particular site is small. This causes large fluctuations in the local spectral density A_{ii} and causes A_{ii} to depend strongly on site energies at distant sites (i.e., to be sensitive to the Thouless boundary condition). This is equivalent to the statement that L_Ω is large and the conductivity is therefore small. Adding an imaginary phonon self-energy tends to damp out the fluctuations in the spectral density and hence enhance the conductivity (cf. Fig. 3). This is equivalent to the statement that the relevant length scale is reduced from L_Ω to l_{ph}, thus enhancing the conductivity.

There is, however, one essential difference between our results and Imry's. We find that for large disorder the addition of even an infinitesimal imaginary self-energy increases the conductivity so that T^* is zero, whereas Imry's argument suggests T^* is finite. It seems to us that Imry's argument is basically correct, but that the inelastic mean free path perhaps enters the problem in a more complicated manner than he suggests.

To illustrate this point it is useful to consider the following relation due to Thouless[40] which is the starting point of the scaling theory of Abrahams *et al.*[30]:

$$\frac{\Delta E(L)}{\delta E(L)} = \frac{2\hbar}{e^2}\, G(L) = \frac{2\hbar}{e^2}\, \sigma(L) L\,. \qquad \text{(A2)}$$

Here, Eq. (A2) is a relation between the conductance G of a cube of length L, δE is the mean spacing of the energy levels of the cube, and ΔE is the average shift in an energy level upon a change in boundary conditions. The second equality of Eq. (A2) serves to define the conductivity of the cube which becomes Ohmic (independent of L) for $L > L_\Omega$.

We note that

$$\delta E(L) \simeq [\rho(\epsilon) L^3]^{-1} = (\rho_i L^3/a^3)^{-1}\,, \qquad \text{(A3)}$$

where ρ_i is the local density of states in a cubic lattice with nearest-neighbor distance a. Then we follow Thouless[40] and note that in the strong-disorder limit $\Delta E(L) = \hbar/t_L$, where t_L is the time it takes an electron to diffuse a distance L ($> L_\Omega$). The time t_L is related to the imaginary part of the electron self-energy, $-\eta$, by the relation $t_L = (L/a)^2 \hbar/\eta$, and consequently

$$\frac{\Delta E(L)}{\delta E(L)} = \frac{L}{a}\, \eta\rho_i\,. \qquad \text{(A4)}$$

From Eqs. (A2) and (A4) we then conclude that the conductivity is

$$\sigma = (e^2/a\hbar)(\eta\rho_i/2)\,. \qquad \text{(A5)}$$

It is interesting to observe that our analytical result [Eq. (6.15), (6.19), and (6.26)] for the conductivity is also proportional to the imaginary part of the electron self-energy in the strong-disorder limit.

As was discussed in previous sections the self-energy is a sum of two terms, $\eta = \xi + \Delta$, where ξ, the dynamic-phonon term, increases, and Δ, the static term, decreases with increasing temperature. If we identify $\Delta\rho_i/2a$ with $1/L_\Omega$ and introduce the inelastic mean free path as $\eta\rho_i/2a = 1/l_{\text{ph}}$ it follows from Eq. (A5) that

$$\sigma = (e^2/\hbar l)\,, \quad l^{-1} = l_{\rm ph}^{-1} + L_\Omega^{-1}\,, \tag{A6}$$

which should be compared to Eq. (A1), If we assume that for $T > T^*$ and $\xi > \Delta$ it follows that $l \simeq l_{\rm ph}$, and we have Imry's result. However, even when $\xi < \Delta$ (at low temperatures), and thus $l \simeq L_\Omega$, it is conceivable that ξ increases more rapidly than Δ decreases with an increase in temperature, i.e., $|d\xi/dT| > |d\Delta/dT|$, which would result in a negative TCR even for $0 < T < T^*$. This is of course the result of the present work, and it is interesting to note that if the new length $l_{\rm ph}$ were to enter the scaling theory of Imry, as suggested by Eq. (A6), the above-mentioned difference between our results might vanish.

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