

Effect of impurity interaction on the Anderson localization

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Anderson localization is reexamined in the presence of interaction between impurities in two and three dimensions. The interaction gives rise to local order or, alternatively, to a correlated impurity probability distribution. This distribution is constructed explicitly with use of mean-field theory for a model system of a disordered binary alloy with one of the components modeling the impurities. The new probability distribution is then used to recalculate perturbatively the conductivity, starting from the metallic limit. When the interaction between impurities is repulsive, the conductivity is found to decrease relative to the noncorrelated case. The results are also analyzed with use of the renormalization group. If short-range interactions are considered, the critical exponents are unchanged but the value of the fixed-point coupling depends on some model parameters, which we relate to the experimental ones. Our results then fit qualitatively well the experimental data obtained for two quite different systems. In both cases, by varying the strength of the local order in a way specific to each experiment, a metal-insulator transition is induced even if, in the absence of any ordering, the system is metallic.

I. INTRODUCTION

According to the theory of Anderson localization,¹ upon increasing the disorder in a metal, the extended electronic states of the system become localized. When this happens, the metallic properties are lost; the system becomes an insulator. This metal-insulator transition, in three dimensions (3D), occurs at a finite value of the disorder. In 1D and 2D, any nonzero value of the disorder induces the transition. In the early discussions on Anderson localization, the electrons were considered to be noninteracting. Electron correlations introduce further complications. In fact the theory becomes so complicated that it is still not fully understood.²

The impurities, which cause the disorder, are generally³ considered to be independently distributed, according to some probability distribution. They interact with the electrons via a static, typically short-range interaction. Physical quantities, like the conductivity, are to be calculated for a given configuration of impurities and averaging over those configurations is to be done at the final stage. It is this quenched averaging which makes the problem complicated, even in the simplest case of independent impurities. On the other hand, if the metal-insulator transition occurs for a finite concentration of impurities, which may be as high as 50%,⁴ it is difficult to imagine how a picture of independent impurities can be correct. Correlations between impurities are bound to be present and play a role. Depending on their range, these correlations may or may not change the universal properties of the Anderson transition. In any case they are important for the interpretation of experimental results. The aim of the present paper is to demonstrate that it is in fact so (in particular, as far as the fixed-point

value of the theory is concerned).

In Ref. 4 it was shown that a metal-insulator transition can be induced by a rearrangement of the atoms, produced by annealing the samples. On the other hand, it has been shown in the past⁵ that local order between impurities may lower the conductivity, alone, independently of any Anderson localization effect. We are going to explain how the argument goes, shortly. The same lowering of the conductivity by local (or short-range) order is also encountered in a very different system, the Bechgaard salts $(\text{TMTSeF})_2\text{SCN}$, where it is experimentally observed⁶ that a short-range incommensurate modulation forms, which tends to localize the electrons and decrease the conductivity. (Here TMTSeF is an abbreviation for tetramethyltetraselenafulvalene.)

In the present work we examine, in 3D and 2D, how local order between the impurities, produced when interactions among them are taken into account, modifies both the Drude value of the conductivity (as was done in 3D in Ref. 5), and also the Anderson-type localization contribution.⁷ More precisely, we calculate the effect of this local order on each term of the standard perturbation theory [in terms of $1/(k_F l)$] used to study localization (k_F stands for the Fermi momentum, l for the mean free path). In this work we only consider noninteracting electrons. We were initially motivated by the experimental result of Ref. 4. However, we believe that the validity of our theory is much broader. It could, for instance, be used in connection with the experiments on pressure-induced metal-insulator transitions⁸ as well as with those of Ref. 6.

Let us first recall the argument concerning the effect of atomic short-range order on the conductivity. The effect of atomic short-range order, produced by the interaction

between the impurities or more generally between any scattering centers, has been investigated, among others, in the early work of Refs. 9, 10, and 5. The model introduced in Ref. 9 for spins in 3D was applied soon after, in Ref. 10, to 3D alloys of nonmagnetic components. The advantage of this simple model was the following: It produced a recurrence formula which gave ordering parameters at increasing distances from given atoms as a function of temperature and interactions. These ordering functions provided an interpolation between the long-range order (if any) and the standard short-range order.¹¹ The resulting formulas were simple enough to be easily incorporated in the calculation of the transport phenomena. As a consequence, deviations from the Drude value σ_0 of the conductivity were obtained due to the local ordering of interacting atoms. These deviations physically resulted from the interference of electronic plane waves scattered by coupled atoms, analogously to the interference of electromagnetic waves propagating through slits in a screen. This interference is constructive or destructive, depending on the nature of the interactions. Later on⁵ a particular case was considered, where the coupling was due to second-order indirect interaction via the electrons, of the Ruderman-Kittel-Kasuya-Yosida (RKKY) type,¹² between two spins in the case of magnetic impurities, or between two excess charges, in the nonmagnetic case.¹³ It was pointed out that the indirect interaction has the same oscillating form as that of the interference factor, so that their product is positive. As a consequence the deviations from the Drude formula are in the sense of *decreasing the conductivity*, at least for weak scatterers.¹⁴ Were it not for the coupling between the impurities, the interference term, by itself, would average to zero and give no contribution (as is the case in the localization problem with independent impurities, where only self-interacting paths survive¹⁵); for coupled impurities instead, all paths contribute.

In most experimental studies on localization, the samples are prepared at high temperature and then quenched (in the following we will call T_0 the quenching temperature). In the existing localization theories, T_0 is implicitly infinite so that the impurities are independent and the local order is absent. But in actual experiments, T_0 is always finite, and thus a local order is present. In systems which atomically order at some temperature T_c , the role of the local order is maximal in the neighborhood of T_c .⁹⁻¹¹

In view of recent developments on the theory of Anderson localization, in a consistent renormalization group (RG) treatment of the problem one should also renormalize the impurity interactions. If the interactions are of short range, the critical exponents are not expected to be changed, whereas the fixed-point value of the disorder parameter will definitively be changed as demonstrated in the following.

Our paper is organized as follows. In Sec. II we calculate in 3D and 2D the correlated distribution function following the ideas of Ref. 10. Section III contains the derivation, by standard technique,^{16,17} of the modified Drude formula via the effect of the normal ladder diagram in the particle-hole channel σ_{NL} ; in Sec. IV we cal-

culate the weak localization contribution through the maximally crossed diagram σ_{MC} in the presence of impurity correlations. In Sec. V we analyze our perturbative result, in particular when the interactions are of the indirect RKKY type. In Sec. VI we repeat the analysis by using the renormalization group. In Sec. VII we discuss our results in connection with the experimental cases of Refs. 4 and 6.

II. THE IMPURITY PROBABILITY DISTRIBUTION IN THE PRESENCE OF LOCAL ORDER BETWEEN SCATTERING ATOMS

In this section we recall the main steps of Ref. 10 by reformulating them in a way convenient for our further discussions. In particular we give explicitly the probability distribution of the impurity configurations in the presence of impurity interactions. Physical quantities, like the conductivity, calculated in Secs. III and IV will have to be averaged over impurity configurations. In doing so, we show that the problem is identical to the one of computing the local order between impurities, or any scattering center, as was done in Ref. 10.

Following Ref. 10, we imagine our system to be a binary alloy. The two components of the alloy, A and B , occupy the N sites of a D -dimensional hypercubic lattice. Let the B component represent the host atoms with concentration $1-c$ and A represent the impurities with concentration c . Both A and B will scatter the conduction electrons. The aim is to determine $P(S_1, S_2, \dots, S_N)$, the probability that at sites $\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N$, the atoms are in states S_1, S_2, \dots, S_N , respectively, where each $S_k = A$ or B . If the atoms are completely uncorrelated, $P(S_1, S_2, \dots, S_N) = P(S_1)P(S_2) \cdots P(S_N)$, and $P(S_k) = c$ or $1-c$, depending on whether $S_k = A$ or B . We want the simplest $P(S_1, S_2, \dots, S_N)$ which, however, contains the correlations between atoms as a consequence of their interactions. We introduce $P(S_k | S_i)$, the conditional probability of finding an atom at lattice site \mathbf{R}_k in state S_k , provided that site \mathbf{R}_i is occupied by an atom in state S_i . We have

$$\lim_{|\mathbf{R}_k - \mathbf{R}_i| \rightarrow \infty} P(S_k | S_i) = P(S_k). \quad (1)$$

From the law of mass action we get

$$\frac{P(A_k | S_i)}{P(B_k | S_i)} \frac{1-c}{c} = \exp - \frac{E}{k_B T} \quad (2)$$

where k_B is the Boltzmann constant. Here A_k (B_k) corresponds to an A (B) atom at site \mathbf{R}_k and E is the energy difference between configurations which differ only by exchanging an A atom at site \mathbf{R}_k with a B atom at infinity from the arbitrary chosen site \mathbf{R}_i . Note that

$$P(B_k | S_i) = 1 - P(A_k | S_i). \quad (3)$$

Within the approximation of Ref. 10 where only nearest-neighbor interactions were considered, in the mean-field approximation, $E = E_1 - E_2$ where

$$\begin{aligned}
E_1 &= \sum_d [V_{AA}P(A_{k+d}|S_i) + V_{AB}P(B_{k+d}|S_i)] \\
&\quad + z[cV_{AA} + (1-c)V_{AB}], \\
E_2 &= \sum_d [V_{AB}P(A_{k+d}|S_i) + V_{BB}P(B_{k+d}|S_i)] \\
&\quad + z[(cV_{AB} + (1-c)V_{BB})].
\end{aligned} \tag{4}$$

\sum_d denotes summation over nearest neighbors at distance d , and z is their number ($k+d$ is the simplified notation for $\mathbf{R}_k + \mathbf{d}$). V_{AA} , V_{BB} , and V_{AB} are the interaction energies between pairs of nearest neighbors, AA , BB , and AB , respectively. Putting (4) back into (2), one obtains a somewhat complicated formula for $P(A_k|S_i)$. However, with

$$W = V_{AA} + V_{BB} - 2V_{AB} \tag{5}$$

one gets, to the lowest order in $W/(k_B T)$,

$$P(A_k|S_i) \simeq c \left[1 - \frac{(1-c)W}{k_B T} \sum_d [P(A_{k+d}|S_i) - c] \right]. \tag{6}$$

Equation (6) is valid for $R_k \neq R_i$. If $R_k = R_i$ one has

$$P(A_k|A_k) = 1, \quad P(A_k|B_k) = 0. \tag{7}$$

The P 's are related to the local order introduced in formula (1) of Ref. 10. All the above formulas so far have been derived in Ref. 10.

The full normalized probability distribution function is constructed from the $P(S_k|S_i)$ as follows:

$$P(S_1, S_2, \dots, S_N) = \frac{1}{N} \sum_{i=1}^N P(S_i) \prod_{\substack{k=1 \\ (k \neq i)}}^N P(S_k|S_i). \tag{8}$$

Equation (8) is then the "minimal" distribution function in the sense that it contains the minimum information about the interaction between the atoms.

Let us now calculate those averages, by means of (8), which will be needed to obtain the conductivity of our system. We assume that the electrons at point \mathbf{r} are affected by a contact potential of the form

$$U(\mathbf{r}) = \sum_k V(S_k) \delta(\mathbf{r} - \mathbf{R}_k), \tag{9}$$

$V(S_k) = V_A$ or V_B . Then the interaction Hamiltonian in the second quantized formalism is

$$H_I = \int d\mathbf{r} U(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}), \tag{10}$$

where $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r})$ are electron creation and annihilation field operators. The conductivity of the system will be calculated using perturbation theory in H_I . Each term of the perturbation series will have to be averaged over the impurity configurations, using (8). This means we will have to calculate $\langle U(\mathbf{r}) \rangle$, $\langle U(\mathbf{r})U(\mathbf{r}') \rangle$, etc. The calculation of $\langle U(\mathbf{r}) \rangle$ is easily performed, using the relation

$$\sum_{S_i=A,B} P(S_i)P(S_k|S_i) = P(S_k). \tag{11}$$

One obtains

$$\langle U(\mathbf{r}) \rangle = [V_A c + V_B (1-c)] \sum_k \delta(\mathbf{r} - \mathbf{R}_k) = U_1. \tag{12}$$

We choose $V_A c + V_B (1-c)$ as the origin of the potentials and therefore in second order will require $\langle [U(\mathbf{r}) - U_1][U(\mathbf{r}') - U_1] \rangle = U_2$. The calculation of U_2 is given in the Appendix. One obtains

$$\begin{aligned}
U_2 &= c(1-c)(V_A - V_B)^2 \frac{1}{N} \\
&\quad \times \sum_k \delta(\mathbf{r} - \mathbf{R}_k) \left[\delta(\mathbf{r}' - \mathbf{R}_k) - \frac{c(1-c)W}{k_B T_0} \right. \\
&\quad \left. \times \sum_d \delta(\mathbf{r}' - \mathbf{R}_k - \mathbf{d}) \right].
\end{aligned} \tag{13}$$

In (13) the temperature T has been replaced by the quenching temperature mentioned in the Introduction. In the weak U limit, when we assume that the scattering of an electron by the same atom more than twice can be neglected¹⁷ we need to retain only U_2 .

Finally let us calculate the effect of U_2 on the one-particle Green's function. We assume that the electronic mean free path l' (defined below), is large. The calculation of the one-particle Green's function to lowest order in $1/(k_F l')$, where k_F is the Fermi momentum, then follows that given in Refs. 16 and 17.

The self-energy to second order in U is given by

$$\Sigma(p, \omega_n) = \sum_{\mathbf{p}'} G(\mathbf{p}', \omega_n) |U(\mathbf{p} - \mathbf{p}')|^2 \tag{14}$$

where

$$\begin{aligned}
|U(\mathbf{p} - \mathbf{p}')|^2 &= c(1-c)(V_A - V_B)^2 \\
&\quad \times \left[1 - \frac{c(1-c)W}{k_B T_0} \sum_d e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{d}} \right],
\end{aligned} \tag{15}$$

$$|\mathbf{p} - \mathbf{p}'| = |\mathbf{q}| = 2k_F \sin(\theta/2). \tag{16}$$

$|U(\mathbf{p} - \mathbf{p}')|^2$ is the Fourier transform of $\langle U(\mathbf{r})U(\mathbf{r}') \rangle$. We recover in (15) the scattering potential modified by local order obtained in Ref. 10. Here ω_n denote the Matsubara frequencies of the electron and θ is the polar angle between the D -dimensional vectors \mathbf{p} and \mathbf{p}' . Later we will require the average of (15) over the direction of \mathbf{d} which will lead to

$$I_D = \sum_d \exp(i\mathbf{q} \cdot \mathbf{d}) = \begin{cases} z \frac{\sin(qd)}{qd} & \text{in 3D,} \\ z J_0(qd) & \text{in 2D.} \end{cases} \tag{17}$$

In (17), J_0 is the Bessel function of the first kind of index zero¹⁸ and, on the right-hand side, q and d denote absolute values. Using (14), the Dyson equation for the Green's function, to lowest order in $1/(k_F l')$, can be solved¹⁷ with the result

$$G^{-1}(\mathbf{p}, \tilde{\omega}_n) = i\tilde{\omega}_n - \xi_p,$$

$$\tilde{\omega}_n = \omega_n + \frac{i}{2\tau'} \text{sgn}(\omega_n), \quad (18)$$

$$\xi_p = \varepsilon_p - \varepsilon_F.$$

Here $\varepsilon_p = p^2/2$ in atomic units (a.u.) and ε_F is the Fermi energy. The elastic scattering time is given by

$$\frac{1}{\tau'} = \begin{cases} \pi N(\varepsilon_F) Nc(1-c)(V_A - V_B)^2 \int_0^\pi d\theta (\sin\theta) \left[1 - \frac{c(1-c)W}{k_B T_0} I_D \right], & 3D \\ N(\varepsilon_F) Nc(1-c)(V_A - V_B)^2 \int_0^{2\pi} d\theta \left[1 - \frac{c(1-c)W}{k_B T_0} I_D \right], & 2D. \end{cases} \quad (19)$$

For independent scatterers ($W=0$), $1/\tau'$ reduces to

$$\frac{1}{\tau_0} = 2\pi N(\varepsilon_F) Nc(1-c)(V_A - V_B)^2. \quad (20)$$

$N(\varepsilon_F)$ is the density of states for one spin direction at the Fermi energy, in a.u.:

$$N(\varepsilon_F) = \begin{cases} \frac{k_F}{2\pi^2}, & 3D \\ \frac{1}{2\pi}, & 2D. \end{cases} \quad (21)$$

With (17) and (16), the angular integrals in (19) can be done and yield

$$\frac{1}{\tau'} = \begin{cases} \frac{1}{\tau_0} \left[1 - \frac{c(1-c)Wz}{k_B T_0} \frac{\sin^2(k_F d)}{(k_F d)^2} \right], & 3D \\ \frac{1}{\tau_0} \left[1 - \frac{c(1-c)Wz}{k_B T_0} J_0^2(k_F d) \right], & 2D. \end{cases} \quad (22)$$

If $W > 0$ it is clear that $1/\tau' < 1/\tau_0$. One finds regions where some atoms A (or B), spread randomly, happen to be surrounded by a first-neighbor shell of B (or A). Such regions are far apart so that $l' = k_F \tau'$ is large than the mean free path corresponding to complete disorder $l_0 = k_F \tau_0$. For $W < 0$, in contrast, the tendency to segregate renders l' smaller than l_0 .

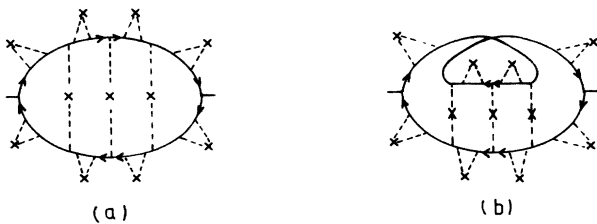


FIG. 1. The two contributions to the conductivity: (a) the one due to the normal ladder, σ_{NL} , (b) the one due to the multiply crossed one, σ_{MC} . Solid lines denote electron Green's functions. Crosses stand for repeated (infinitely many times) correlated impurity scatterings.

III. MODIFICATIONS TO THE DRUDE FORMULA OF THE CONDUCTIVITY DUE TO THE COUPLINGS BETWEEN SCATTERING ATOMS: CALCULATION OF σ_{NL}

In this section we calculate how the usual Drude expression σ_0 of the conductivity is modified when the scattering atoms interact via the coupling W . We thus compute the normal ladder (NL) diagram of Fig. 1(a), yielding the conductivity contribution σ_{NL} . To do so we need to compute first the current vertex correction in the particle hole channel Λ of Fig. 2(a) as usual:^{16,17}

$$\Lambda(\mathbf{p}, \tilde{\omega}_{n+\nu}; \mathbf{p}, \tilde{\omega}_n) = \mathbf{p} + \int \frac{d^d \mathbf{p}'}{(2\pi)^d} G_0(\mathbf{p}', \tilde{\omega}_{n+\nu}) G_0(\mathbf{p}', \tilde{\omega}_n) \times \Lambda(\mathbf{p}', \tilde{\omega}_{n+\nu}; \mathbf{p}', \tilde{\omega}_n) \times |U(\mathbf{p}' - \mathbf{p})|^2. \quad (23)$$

We choose $\omega_\nu > 0$. Writing

$$\Lambda(\mathbf{p}, \tilde{\omega}_{n+\nu}; \mathbf{p}, \tilde{\omega}_n) = \mathbf{p}\gamma \quad (24)$$

and multiplying both sides of (23) by \mathbf{p} one obtains, with $|\mathbf{p}| \sim |\mathbf{p}'| \sim k_F$ with k_F the Fermi momentum,

$$k_F^2 \gamma = k_F^2 + k_F^2 \gamma \int \frac{d^d \mathbf{p}'}{(2\pi)^d} G_0 G_0 |U|^2 \cos\theta \quad (25)$$

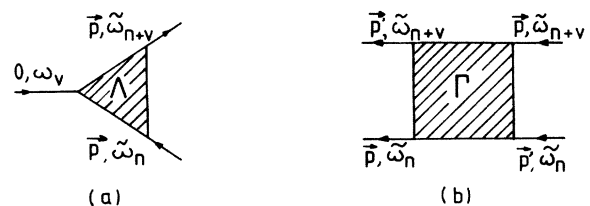


FIG. 2. Vertex contributions entering in the calculation of the conductivity: (a) Λ implied in σ_{NL} [Eq. (23)], (b) Γ implied in σ_{MC} [Eq. (38)].

where $\mathbf{p} \cdot \mathbf{p}' = p_F^2 \cos\theta$.

One then obtains

$$\gamma = \left[1 - \frac{1}{\tau''} \frac{\Theta(\omega_{n+v})\Theta(-\omega_n)}{\omega_v + \tau'^{-1}} \right]^{-1}, \tag{26}$$

$$\frac{1}{\tau''} = \begin{cases} \pi N(\epsilon_F) \int_0^\pi |U|^2 \sin\theta \cos\theta d\theta, & \text{3D} \\ N(\epsilon_F) \int_0^{2\pi} |U|^2 \cos\theta d\theta, & \text{2D} . \end{cases} \tag{27}$$

Using $|U|^2$ derived in the preceding section, with $V = V_A - V_B$ one gets

$$\frac{1}{\tau''} = \begin{cases} \pi N(\epsilon_F) Nc(1-c)V^2 \int_0^\pi d\theta \cos\theta \sin\theta \left[1 - \frac{c(1-c)Wz}{k_B T_0} \frac{\sin[2k_F d \sin(\theta/2)]}{2k_F d \sin(\theta/2)} \right], & \text{3D} \\ N(\epsilon_F) Nc(1-c)V^2 \int_0^{2\pi} d\theta \cos\theta \left[1 - \frac{c(1-c)Wz}{k_B T_0} J_0(2k_F d \sin(\theta/2)) \right], & \text{2D} . \end{cases} \tag{28}$$

The calculations are straightforward using standard integrals.¹⁸ We give the result under the form needed in (26) and in the following:

$$\frac{1}{\tau'} - \frac{1}{\tau''} = \begin{cases} \frac{1}{\tau_0} \left\{ 1 + \frac{c(1-c)Wz}{k_B T_0} \frac{1}{(k_F d)^2} \left[\left[\cos(k_F d) - \frac{\sin(k_F d)}{k_F d} \right]^2 - \sin^2(k_F d) \right] \right\}, & \text{3D} \\ \frac{1}{\tau_0} \left\{ 1 + \frac{c(1-c)Wz}{k_B T_0} [J_1^2(k_F d) - J_0^2(k_F d)] \right\}, & \text{2D} . \end{cases} \tag{29}$$

J_0 and J_1 are the Bessel functions of the first kind of respective indices zero and one.^{18,19}

We now calculate the “normal ladder” conductivity σ_{NL} [diagram of Fig. 1(a)]. The current-current correlation function K_{xx} projected on the x axis is given by

$$K_{xx} = -2T \sum_n \int \frac{d^d \mathbf{p}}{(2\pi)^d} G_0(\mathbf{p}, \bar{\omega}_{n+v}) G_0(\mathbf{p}, \bar{\omega}_n) (\mathbf{\Lambda} \cdot \mathbf{p})_{xx} . \tag{30}$$

Using (24) and (25),

$$\sigma_{NL} = \lim_{\omega \rightarrow 0} \frac{K_{xx}(\omega) - K_{xx}(0)}{i\omega}, \tag{31}$$

$\omega = i\omega_v$.

One straightforwardly obtains

$$\sigma_{NL} = \frac{N_{\text{eff}}}{(\tau')^{-1} - (\tau'')^{-1}} \tag{32}$$

where N_{eff} is the effective number of electrons per unit volume:

$$N_{\text{eff}} = \begin{cases} k_F^3 / (3\pi^2), & \text{3D} \\ k_F^2 / 2\pi, & \text{2D} . \end{cases} \tag{33}$$

Then in terms of the Drude formula σ_0 corresponding to independent scatterers (in a.u.),

$$\sigma_0 = N_{\text{eff}} \tau_0 . \tag{34}$$

One gets, to first order in $W/(k_B T_0)$,

$$\sigma_{NL} = \begin{cases} \sigma_0 \left\{ 1 - \frac{zc(1-c)W}{k_B T_0} \frac{1}{(k_F d)^2} \left[\left[\cos(k_F d) - \frac{\sin(k_F d)}{k_F d} \right]^2 - \sin^2(k_F d) \right] \right\}, & \text{3D} \\ \sigma_0 \left\{ 1 - \frac{zc(1-c)W}{k_B T_0} [J_1^2(k_F d) - J_0^2(k_F d)] \right\}, & \text{2D} . \end{cases} \tag{35}$$

One easily verifies that the 3D result is exactly the one obtained in Ref. 10.

We mention the approximate forms of (35) which are valid when $k_F d \gg 1$. Using asymptotic expansions of the Bessel functions¹⁹ in the 2D case, we obtain

$$\sigma_{\text{NL}} \underset{k_F d \gg 1}{\sim} \begin{cases} \sigma_0 \left[1 - \frac{c(1-c)Wz}{k_B T_0} \frac{\cos(2k_F d)}{(k_F d)^2} \right], & 3\text{D} \\ \sigma_0 \left[1 + \frac{c(1-c)Wz}{k_B T_0} \frac{2}{\pi} \frac{\sin(2k_F d)}{(k_F d)} \right], & 2\text{D} . \end{cases} \quad (36)$$

These formulas will be useful in Sec. V, where we discuss the case when W is given by the indirect exchange interaction of the RKKY type. The asymptotic forms for W then are proportional, respectively, to $\cos(2k_F d)/(k_F d)^3$ in 3D and $-\sin(2k_F d)/(k_F d)^2$ in 2D so that the overall σ_{NL} in (36) is decreased compared to σ_0 , whatever $k_F d$ ($\gg 1$) is.

IV. MODIFICATIONS OF THE LOCALIZATION CONTRIBUTION TO THE CONDUCTIVITY DUE TO THE COUPLINGS BETWEEN SCATTERING ATOMS: CALCULATION OF σ_{MC}

We now turn to the calculation of the multiply crossed diagram of Fig. 1(b) usually responsible for the localization of the electrons.¹ As is well known and clear in Fig. 1(b), one first needs to calculate the ladder correction Γ in the particle-particle channel of Fig. 2(b). Writing for simplicity,

$$|U(\mathbf{p}' - \mathbf{p})|^2 = Z [1 + \delta Z (|\mathbf{p}' - \mathbf{p}|)] . \quad (37)$$

We write the Bethe-Salpeter equation for Γ as follows:

$$\begin{aligned} \Gamma(\mathbf{p}, \mathbf{p}', \bar{\omega}_{n+\nu}; \mathbf{p}', \mathbf{p}, \bar{\omega}_n) = & Z [1 + \delta Z (|\mathbf{p}' - \mathbf{p}|)] + \int \frac{d^d \mathbf{k}}{(2\pi)^d} G_0(\mathbf{k}, \bar{\omega}_{n+\nu}) G_0(\mathbf{p} + \mathbf{p}' - \mathbf{k}, \bar{\omega}_n) Z [1 + \delta Z (|\mathbf{k} - \mathbf{p}|)] \\ & \times \Gamma(\mathbf{k}, \mathbf{p}', \bar{\omega}_{n+\nu}; \mathbf{p} + \mathbf{p}' - \mathbf{k}, \mathbf{p}, \bar{\omega}_n) . \end{aligned} \quad (38)$$

Then we iterate the above equation, retaining terms only of first order in W/T_0 , as it has been done in the preceding section. One finally arrives at

$$\Gamma = \frac{Z}{1 - ZB} - \frac{c(1-c)W}{k_B T_0} Z \sum_{\mathbf{d}} \left[e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{d}} + \frac{Z}{1 - ZB} [e^{i\mathbf{p}' \cdot \mathbf{d}} A(\mathbf{d}) + e^{-i\mathbf{p} \cdot \mathbf{d}} A(-\mathbf{d})] + \frac{Z^2}{(1 - ZB)^2} A(\mathbf{d}) A(-\mathbf{d}) \right] \quad (39)$$

with

$$A(\pm \mathbf{d}) = e^{\pm i(\mathbf{p} + \mathbf{p}') \cdot \mathbf{d}} \int \frac{d^d \mathbf{k}}{(2\pi)^d} G_0(\mathbf{k}, \bar{\omega}_{n+\nu}) G_0(\mathbf{p} + \mathbf{p}' - \mathbf{k}, \bar{\omega}_n) e^{\pm i\mathbf{k} \cdot \mathbf{d}} , \quad (40)$$

$$B = \int \frac{d^d \mathbf{k}}{(2\pi)^d} G_0(\mathbf{k}, \bar{\omega}_{n+\nu}) G_0(\mathbf{p} + \mathbf{p}' - \mathbf{k}, \bar{\omega}_n) . \quad (41)$$

Note, however, that in (39), terms of first order in Z have been taken care of in the preceding section. We then define Γ' as the particle-particle ladder Γ without those terms. Diagrammatically, the first-order corrections in δZ to Γ' are given in Fig. 3. B can be easily computed to yield

$$B(\mathbf{p} + \mathbf{p}', \omega_\nu) = \frac{2\pi \Theta(\omega_{n+\nu}) \Theta(-\omega_n) N(\epsilon_F)}{\omega_\nu + \frac{1}{\tau}} \left[1 - \frac{1}{D} k_F^2 |\mathbf{p} + \mathbf{p}'|^2 (\tau')^2 \right] \quad (42)$$

(recall that D is the dimension). In (42) $1/\tau'$ is given by formula (19). Note that in order to obtain the full expression for Γ valid to lowest order in δZ , B , in the first term of (39), has to be further expanded using (19) and (20).

The calculation of $A(\pm \mathbf{d})$ requires a tedious but straightforward algebra. Defining

$$\mathbf{p} + \mathbf{p}' = \mathbf{Q}, \quad \alpha = k_F d , \quad (43)$$

$$\begin{aligned} A(\pm \mathbf{d}) = & e^{\mp i\mathbf{Q} \cdot \mathbf{d}} \frac{2\pi N(\epsilon_F)}{\omega_\nu + \frac{1}{\tau_0}} \left[\frac{\sin \alpha}{\alpha} \mp \frac{k_F Q}{\omega_\nu + \frac{1}{\tau_0}} \frac{\mathbf{Q} \cdot \mathbf{d}}{Qd} \left[\frac{\cos \alpha}{\alpha} - \frac{\sin \alpha}{\alpha^2} \right] \right. \\ & \left. - \frac{1}{\left[\omega_\nu + \frac{1}{\tau_0} \right]^2} k_F^2 Q^2 \left[-\frac{\cos \alpha}{\alpha^2} + \frac{\sin \alpha}{\alpha^3} + \frac{(\mathbf{Q} \cdot \mathbf{d})^2}{Q^2 d^2} \left[\frac{\sin \alpha}{\alpha} + \frac{3 \cos \alpha}{\alpha^2} - \frac{3 \sin \alpha}{\alpha^3} \right] \right] \right] , \quad 3\text{D} \end{aligned} \quad (44)$$

$$A(\pm d) = e^{\mp i\mathbf{Q}\cdot\mathbf{d}} \frac{2\pi N(\epsilon_F)}{\omega_v + \frac{1}{\tau_0}} \left[J_0(\alpha) \pm \frac{k_F Q}{\omega_v + \frac{1}{\tau_0}} \frac{\mathbf{Q}\cdot\mathbf{d}}{Qd} J_1(\alpha) - \frac{1}{\left[\omega_v + \frac{1}{\tau_0}\right]^2} k_F^2 Q^2 \left[\frac{J_1(\alpha)}{\alpha} - \frac{(\mathbf{Q}\cdot\mathbf{d})^2}{Q^2 d^2} \left[\frac{2J_1(\alpha)}{\alpha} - J_0(\alpha) \right] \right] \right], \quad 2D. \quad (45)$$

The above expressions are valid up to second order in Q . With all these ingredients, we can now compute the contribution σ_{MC} to the conductivity given by the multiply crossed diagram of Fig. 1(b). The contribution of the multiply crossed diagram to the current-current correlation function reads

$$K_{xx} = -2T \sum_n \int \frac{d^d p'}{(2\pi)^d} \int \frac{d^d p_x}{(2\pi)^d} p_x p'_x \Gamma'(\mathbf{p} + \mathbf{p}', \omega_v) G_0(\mathbf{p}, \bar{\omega}_{n+v}) G_0(\mathbf{p}, \bar{\omega}_n) G_0(\mathbf{p}', \bar{\omega}_{n+v}) G_0(\mathbf{p}', \bar{\omega}_n). \quad (46)$$

We use (43) and the diffusion coefficient

$$D_0 = \frac{k_F^2 \tau_0}{D}. \quad (47)$$

Finally we obtain, for σ_{MC} ,

$$\sigma_{MC} = \begin{cases} -\frac{k_F^2}{3} \frac{1}{\pi^3} 2\pi N(\epsilon_F) \tau'^3 \int_0^{1/l'} dQ Q \Gamma'(\omega_v=0), & 3D \\ -\frac{k_F^2}{2} \frac{1}{\pi^2} 2\pi N(\epsilon_F) \tau'^3 \int_{1/L}^{1/l'} dQ Q \Gamma'(\omega_v=0), & 2D. \end{cases} \quad (48)$$

As usual,¹ the lower cutoff in 2D involves the macroscopic linear size L of the system. $\Gamma'(\omega_v=0)$ in (48) is given by

$$\Gamma'(\omega_v=0) = \begin{cases} \frac{1}{2\pi N(\epsilon_F) \tau_0^2} \frac{1}{D_0 Q^2} \left[1 + \frac{zc(1-c)W}{k_B T_0} \left[\frac{\cos(2\alpha)}{\alpha^2} - \frac{\sin(2\alpha)}{\alpha^3} + \frac{1-\cos(2\alpha)}{2\alpha^4} - 2\frac{\sin^2\alpha}{\alpha^2} \right] \right], & 3D \\ \frac{1}{2\pi N(\epsilon_F) \tau_0^2} \frac{1}{D_0 Q^2} \left[1 + \frac{zc(1-c)W}{k_B T_0} [J_1^2(\alpha) - 3J_0^2(\alpha)] \right], & 2D. \end{cases} \quad (49)$$

We wish to make here the following remark: in contrast with what could be thought *a priori*, the $(1-ZB)^2$ denominator in the fourth term of (39) cancels with a similar term coming from the expansion to first order in $W/(k_B T_0)$ of the first term. This remark is crucial since a term in $(1-ZB)^{-1}$ in Γ' involves the usual pole $(D_0 Q^2 + \omega_v)^{-1}$ while $(1-ZB)^{-2}$ would imply $(D_0 Q^2 + \omega_v)^{-2}$, i.e., a stronger singularity than the one usually involved in localization theory. In other words, at least to first order in $W/(k_B T_0)$, the singularity remains of the same kind as for independent scatterers. In (48) τ' has to be expressed by (19) and (20); $l' = k_F \tau'$ and $l_0 = k_F \tau_0$. Finally,

$$\sigma_{MC} = \begin{cases} -\frac{1}{\pi^3 l_0} \left\{ 1 + \frac{zc(1-c)W}{k_B T_0} \frac{1}{(k_F d)^2} \left[\left[\cos(k_F d) - \frac{\sin(k_F d)}{k_F d} \right]^2 - \sin^2(k_F d) \right] \right\}, & 3D \\ -\frac{1}{\pi^2} \left[1 + \frac{zc(1-c)W}{k_B T_0} J_1^2(k_F d) \right] \ln \frac{L}{l_0}, & 2D. \end{cases} \quad (50)$$

Note that in the absence of coupling between the scattering atoms, for $W=0$, one recovers the localization formulas:¹

$$\sigma_{MC}(W=0) = \begin{cases} -\frac{1}{\pi^3 l_0}, & 3D \\ -\frac{1}{\pi^2} \ln \frac{L}{l_0}, & 2D. \end{cases} \quad (51)$$

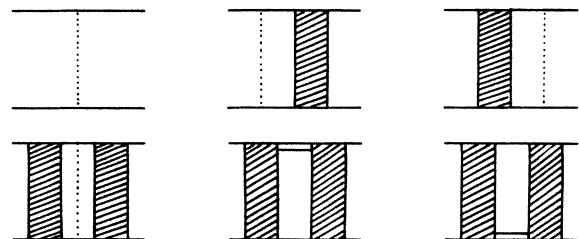


FIG. 3. Diagrammatic representation of the first-order corrections in δZ to Γ' . The dotted line denotes δZ ; the shaded blocks correspond to the direct ladder, calculated with $\delta Z=0$. The single line stands for the Green's function with $\delta Z=0$, whereas the double line is the first correction in δZ .

This perturbative result for the total conductivity will be analyzed in the next section.

**V. ANALYSIS OF THE PERTURBATIVE RESULT
OBTAINED FOR σ_{total}
AND THE PARTICULAR CASE
WHERE THE ATOMS INTERACT
VIA A RKKY-TYPE W**

The results for σ_{NL} given by (35) and σ_{MC} given by (50) are the key results of our paper. The total conductivity σ_{total} is then given by

$$\sigma_{\text{total}} = \sigma_{\text{NL}} + \sigma_{\text{MC}}. \quad (52)$$

The local order effect between the atoms will depend on the strength and sign of W and on the oscillating functions of $k_F d$. Note, however, that in 2D the sign of the localization term σ_{MC} only depends on the sign of W . This will be of importance in the next section. In 3D, it is interesting to point out that it is the same oscillating function of $k_F d$ which altogether decreases (increases) σ_{NL} with respect to σ_0 , for $W > 0$ (< 0) and enhances (diminishes) the localization term σ_{MC} . This is not so in 2D where a different oscillating function enters ($J_1^2 - J_0^2$ in σ_{NL} compared to J_1^2 alone in σ_{MC}).

So far W was not made explicit. It may contain several contributions: direct (of chemical origin for instance), as well as indirect ones (mediated by the electrons). It was given in formula (5) in terms of the three quantities V_{AA} , V_{BB} , and V_{AB} . In fact for a binary alloy undergoing an order-disorder transition at some temperature T_c , W is related to T_c through $T_c = zc(1-c)W$, at a second-order transition within the Bragg-Williams approximation,¹¹ for two independent sublattices. In that case, W is positive, i.e., two atoms of the same kind repel each other, while different atoms attract one another. A measure of W is then given once T_c is known. In contrast, when W is negative, there is no ordering transition, the system tends to segregate: the atoms of the same kind attract each other, while different atoms repel. Various contributions may enter in the values of V_{AA} , V_{BB} , and V_{AB} . Our purpose is not to enter into these details here. We wish, in the present section, to concentrate on one particular case, where the A (and B) atoms can be considered as point charges interacting with their neighbors not directly but via an interaction carried by the electrons. Such an interaction is analogous to the Ruderman-Kittel-Kasuya-Yosida (RKKY) indirect interaction between magnetic impurities.¹² Then, as is well known,¹² a second-order perturbation calculation gives, in 3D,

$$W(d) = \omega_{3D} \left[-\frac{\sin(2k_F d) - 2k_F d \cos(2k_F d)}{(2k_F d)^4} \right], \quad (53)$$

where the oscillating function of $2k_F d$ is just the Fourier transform of the Lindhard function:²⁰ ω_{3D} (as well as ω_{2D} used below) is proportional to $(1/\epsilon_F)(J_{eA}^2 + J_{eB}^2 - 2J_{eA}J_{eB})$ where the J 's are the interaction energies between the electrons and the A (or the B) charges. Therefore ω_{3D} (ω_{2D}) is a positive quantity. The RKKY calculation can be easily performed in 2D (Ref. 21) and yields

$$W(d) = \omega_{2D} [J_0(k_F d)N_0(k_F d) + J_1(k_F d)N_1(k_F d)]; \quad (54)$$

N_0 and N_1 are the Bessel functions of the second kind¹⁸ of respective indices zero and one. Note that compared to the spin problem involving the RKKY interaction, in case of charged impurities, an additional complication arises. This is related to the fact that charges are screened, whereas spins are not. As a result the indirect interaction is slightly changed.^{5,13} However, when $k_F d \gg 1$ (which is the case in normal metals even when d is the nearest-neighbor distance), the asymptotic formulas for the indirect interactions are given both in the spin and the charge cases by⁵

$$W(d) \underset{k_F d \gg 1}{\approx} \omega_{3D} \frac{\cos(2k_F d)}{(2k_F d)^3}, \quad 3D. \quad (55)$$

Similarly in 2D, using asymptotic expansions of the Bessel functions:¹⁹

$$W(d) \underset{k_F d \gg 1}{\approx} -\omega_{2D} \frac{\sin(2k_F d)}{(2k_F d)^2}, \quad 2D. \quad (56)$$

In our case of charged impurities the prefactor ω 's will be different from the expressions given above in the RKKY case.

Then our formulas (36) for σ_{NL} (where we retain the leading term in $1/k_F d$ in the interference contribution), combined with (55) and (56) give

$$\sigma_{\text{NL}} \underset{k_F d \gg 1}{\sim} \begin{cases} \sigma_0 \left[1 - \frac{c(1-c)z}{k_B T_0} \omega_{3D} \frac{\cos^2(2k_F d)}{(2k_F d)^5} \right], & 3D \\ \sigma_0 \left[1 - \frac{c(1-c)z}{k_B T_0} \omega_{2D} \frac{\sin^2(2k_F d)}{(2k_F d)^3} \right], & 2D. \end{cases} \quad (57)$$

Then σ_{NL} is always decreased compared to σ_0 , whatever the value of $k_F d \gg 1$ is. The 3D result has already been found and discussed in Ref. 5, as mentioned earlier. Here we just showed that the same tendency holds in 2D as well.

Combining (57) with (50) and (55), in 3D to leading order in $1/k_F d$, we get

$$\sigma_{\text{total}} = \sigma_0 \left[1 - \frac{c(1-c)z}{k_B T_0} \omega_{3D} \frac{\cos^2(2k_F d)}{(2k_F d)^5} - \frac{3}{4\pi(\epsilon_F \tau_0)^2} \left[1 + \frac{c(1-c)z}{k_B T_0} \omega_{3D} \times \frac{\cos^2(2k_F d)}{(2k_F d)^5} \right] \right]. \quad (58)$$

Equation (58) shows that the local order between the atoms in 3D always decreases σ_{NL} compared to σ_0 (for $\omega_{3D} > 0$) whatever $k_F d \gg 1$ is and renders σ_{MC} more negative. In other words, the presence of a finite interaction of RKKY type enhances the Anderson localization effect. In 2D instead, while the local order decreases σ_{NL} , as it does in 3D, its effect on σ_{MC} remains oscillating.

VI. RENORMALIZATION GROUP ANALYSIS

In this section, we analyze the results of Secs. III and IV using the renormalization group (RG) approach. There are a number of ways the RG can be applied to the Anderson localization problem in the absence of interactions (some of the approaches are listed in Refs. 22–26). For concreteness we are going to use the method of Ref. 26. In that work the RG equations were derived by parametrizing the transformation by the choice of the normalization point of the “vertex” function, defined by

$$D_R = D_0 \Pi . \quad (59)$$

Here D_R is the renormalized diffusion constant. The function Π depends on L . The normalization point is defined by

$$\Pi'(L = \lambda) = \Pi'_{\text{NP}} = 1 , \quad (60)$$

where

$$\begin{aligned} \Pi' &= Z_\lambda \Pi(LZ_\lambda^{-1}, \sigma' Z_\lambda) , \\ \sigma' &= Z_\lambda^{-1} g_0 . \end{aligned} \quad (61)$$

In (61) g_0 is the dimensionless conductance used as the coupling constant of the theory and Z_λ is independent of L . The parameter of the transformation leading from normalization point λ to λ' is

$$Z_{\lambda'/\lambda} = Z_{\lambda'} / Z_\lambda . \quad (62)$$

The RG equations are derived in the standard way (for details see Ref. 26 in terms of $Z_{\lambda'/\lambda}$). In $2 + \epsilon$ dimensions the equation for σ^* , the fixed-point coupling, is

$$\sigma^* \left[-\epsilon + \left. \frac{\partial Z_{\lambda'/\lambda}^{-1}(\sigma^*)}{\partial \lambda'/\lambda} \right|_{\lambda'=\lambda} \right] = 0 . \quad (63)$$

The nontrivial value of σ^* is obtained by calculating $Z_{\lambda'/\lambda}$ in perturbation theory. Using (50) (which is enough to lowest order in ϵ) (63) leads to

$$\sigma^* = \frac{1}{\epsilon} \left[1 + \frac{zc(1-c)W}{k_B T_0} J_1^2(k_F d) \right] . \quad (64)$$

A few comments are necessary concerning this result. First, the perturbative results obtained in the preceding section for the maximally crossed diagram are valid only in the weak scattering limit. This means the concentration of impurities c has to be small, and $1 - c \sim 1$ in (64) (and in all the previous formulas for σ_{MC}). Secondly, as explained in the Introduction, in a consistent RG theory the interaction between impurities should also be renormalized. If only the direct interactions are considered, this, however, may not be so. W and T_0 enter our formulas for the conductivity through the averaging process. If W is independent of the electronic motion the dynamics of the impurities gives rise only to a correlated probability distribution. The electronic properties are recalculated with this modified distribution. The interaction between the impurities parametrizes their distribution. (For each W there is another distribution.) Clearly, in this case, W does not have to be renormalized. On the

other hand, if W includes an indirect RKKY-type interaction, it certainly has to be renormalized (at least its indirect part). The RKKY interaction between the impurities is mediated by the electrons. If these become localized, the RKKY interaction is strongly modified. This means the impurity distribution and the electronic motion are coupled. Besides the fixed point (64) a fixed-point probability distribution should be derived, which still might be parametrized by the direct interaction and T_0 . This complicated renormalization is not carried out in the present paper.

As stated earlier we do not expect the universal properties of the Anderson transition to change in the presence of short-range correlations between impurities. Indeed, the critical exponents are unchanged in the present calculation. In contrast, if either long-range or marginal indirect interactions are involved, the critical exponents might change. An example of marginality is the RKKY-type interaction given by (55) and (56) with d replaced by $|\mathbf{R}_i - \mathbf{R}_j|$, the distance between impurities at sites \mathbf{R}_i and \mathbf{R}_j . The result (64) allows us to interpret a number of experimental results, as will be demonstrated in the next section.

VII. DISCUSSION AND COMPARISON WITH EXPERIMENTS

Our theoretical study of the effect of short-range order on the conductivity was first motivated by the experimental results of Ref. 4. In that reference it was shown that a metal-insulator transition can be induced by annealing. $\text{Al}_x\text{Ge}_{1-x}$ samples ($0.7 > x > 0.4$) were prepared by coevaporation at 5 K, still in the metallic regime, although in an atomically disordered amorphous state. The metal-insulator transition was subsequently studied by measuring the conductivity down to 0.25 K. In this way the transition was established to take place for $x_0 \sim 0.475$. In another series of experiments the samples were annealed to some higher temperatures, and then quenched again to 5 K. It was found that this procedure, at a given value of the annealing temperature T_a (dependent on x), induced the metal-insulator transition. This occurred even in samples which initially, when prepared at 5 K, were metallic. The more metallic the samples were at 5 K (the bigger was x) the higher T_a values were required to induce the metal-insulator transition. The explanation of this interesting phenomenon, as given in Ref. 4, was based on the assumption that annealing increased the microscopic disorder. At T_a the disorder reaches locally its critical value and the metal-insulator transition takes place. The critical value itself (fixed point of the disorder) was assumed in Ref. 4 to be independent of annealing.

In what follows, using the results of the previous sections, we attempt to give an alternative explanation of these experimental findings. The metal-insulator transition induced by annealing, according to our view, is a result of a microscopic mechanism, quite different from the one proposed in Ref. 4. It is reasonable to assume²⁷ that, upon annealing, the thermal motion (even modest) is sufficient for the atoms to locally rearranged in an ener-

getically more favorable state, so that a short-range order tends to form. The higher T_a , the more effective are the interactions, i.e., the short-range ordering. In our model instead, the short-range order is more efficient for lower values of T_0 . There are a number of differences between the experiments of Ref. 4 and our basic hypotheses: (a) the initial disorder is established in a different way (co-evaporation at low T in Ref. 4, compared to quenching from a high-temperature T_0 in our model); (b) the $\text{Al}_x\text{Ge}_{1-x}$ samples have an amorphous structure while we are supposed to deal with a crystal with a well-defined nearest-neighbor distance d and a fixed number of nearest neighbors z ; and (c) increasing T_a in Ref. 4 corresponds, as mentioned above, to decreasing T_0 in our case (the simplest relation between T_a and T_0 may be $T_a \propto 1/T_0$). Due to these differences, it is not possible to make a quantitative comparison between our results and those of Ref. 4. However, it is clear that, qualitatively, they fit the experimental tendency well. As shown in the present paper, interactions between impurities give rise to a short-range order which may enhance the localization effect. Our perturbative result in 3D, Eq. (58), indicates that upon annealing (if we use the above correspondence $T_a \sim 1/T_0$), for fixed c [$= (1-x)$ in Ref. 4] the system loses its metallic properties. In $2+\epsilon$ dimensions, using the results of the RG analysis of Sec. VI, we obtain that σ^* , for fixed c , increases with T_a [Eq. (64) with $W > 0$]. In other words, compared with an initially disordered state yielding a sample in the metallic regime, the establishment of a small amount of short-range (local) order may be sufficient to switch the sample to scale towards an insulator. The fact that the fixed point depends continuously on T_a (or T_0) might seem surprising at first sight. In view of the discussion in Sec. VI, it is not so. T_0 (or T_a) parametrizes the impurity distribution function. The result that the value of the fixed point depends on the probability distribution used to calculate the quenched average quantities is quite reasonable. The critical exponents, on the other hand, are the same for the annealed system as for the original one. This is another manifestation of universality.

To conclude this part, the effect of annealing is to allow for rearrangement. By this, the interaction between scatterers is activated and a correlated impurity distribution is obtained. This distribution depends continuously on T_0 (T_a) and therefore so does the fixed-point value of the disorder parameter. If the scatterers repel each other²⁸ [$W > 0$ in (64)] the critical value σ^* of the disorder is increased. This means that the annealing procedure allows the metal-insulator transition to occur at a smaller c value than in the absence of annealing. These findings are in complete qualitative agreement with the experimental results of Ref. 4.

Similar remarks apply, still qualitatively, to the experimental results of Refs. 6 on a Bechgaard salt $(\text{TMTSeF})_2\text{SCN}$. This material is metallic at high T . However, a well-defined cusp in the T dependence of the resistivity is observed around 95 K. The behavior of the resistivity $\rho(T)$ changes at this temperature. Above it, $\rho(T)$ has a metallic character, whereas below, $\rho(T)$ corresponds to the hopping mechanism of Mott. These experi-

mental findings correspond to a metal-insulator transition in the following sense: if the system is quenched from $T > 95$ K to $T=0$, the residual conductivity is finite; quenching from $T < 95$ K, on the other hand, results in a vanishing conductivity, i.e., an insulator. In Ref. 6, x-ray studies demonstrate the formation of a short-range incommensurate modulation for $T > 95$ K, strengthened when T approaches that temperature from above. The source of the modulation is not understood at present. However, it is clear experimentally that such a short-range ordering is at the origin of the transition. This observation, qualitatively, can be easily understood using our theory. The short-range order increases with decreasing T , just as it does in our model (when T_0 decreases). In this sense, our model is more directly applicable to the system of Ref. 6 than to that of Ref. 4. According to our theory, the strength of the short-range order, achieved at around 95 K, is sufficient to drive the system insulating in the above sense. In other words, at $T \sim 95$ K, σ^* in Eq. (64) now exceeds (or equals) the initial disorder (see Fig. 4). It has also been found in Ref. 6 that application of 2 kbar pressure stabilizes the metallic state down to low temperatures. We believe the effect of this pressure is to push σ_0 in Fig. 4 to such a high value that cannot be reached by a shift of σ^* due to short-range order. To check this conjecture, the experiments should be performed systematically as a function of pressure between 0 and 2 kbar. As a conclusion we think that the experimental result of Ref. 6 is another example of electron localization driven by short-range order, whatever is its origin.

As far as the theory is concerned, it would be interesting to examine how the range of the interaction between impurities may affect the scaling behavior of the system. In particular, if these interactions introduce further scaling parameters, the critical exponents would most likely be changed.

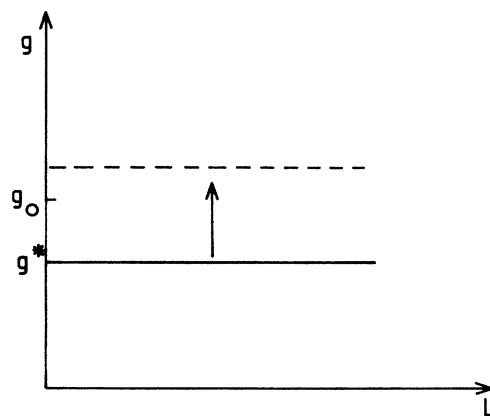


FIG. 4. The dimensionless conductance fixed point σ^* above (below) which the system scales to a metal (insulator) when the linear dimension L increases. σ_0 is the initial value of the conductance at the microscopic length scale. The arrow shows how the local order shifts the phase boundary, when $W > 0$ [according to Eq. (64)].

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APPENDIX

In order to obtain $U_2 = \langle [U(r) - U_0][U(r') - U_0] \rangle$, we have to calculate $\langle [V(S_{k_1}) - V_0][V(S_{k_2}) - V_0] \rangle$, where

$$V_0 = V_A c + V_B(1-c). \quad (\text{A1})$$

Let us then calculate $\langle V(S_{k_1})V(S_{k_2}) \rangle$. Since U_2 involves summation over k_1 and k_2 , we have to distinguish two cases according to whether $R_{k_1} = R_{k_2}$ or $R_{k_1} = R_{k_2} + d$. It is easy to see that for any other relation between R_{k_1} and R_{k_2} , the corresponding contribution to U_2 will be zero. The case $R_{k_1} = R_{k_2}$ requires essentially the same calculation as U_1 . One obtains

$$\langle V^2(S_k) \rangle - V_0^2 = \frac{1}{N}(V_A - V_B)^2 c(1-c). \quad (\text{A2})$$

The second case is considerably more complicated and will be worked out in detail. According to the definition of $P(S_1, S_2, \dots, S_N)$ given by (8)

$$\begin{aligned} \langle V(S_k)V(S_{k+d}) \rangle &= \frac{1}{N} \sum_{\{S\}} V(S_k)V(S_{k+d}) \\ &\quad \times \sum_i P(S_i) \prod_{l(\neq i)} P(S_l | S_i) \\ &= K_1 + K_2 \end{aligned} \quad (\text{A3})$$

where

$$K_1 = \frac{1}{N} \sum_{\{S\}} V(S_k)P(S_k)V(S_{k+d})P(S_{k+d} | S_k), \quad (\text{A4})$$

$$\begin{aligned} K_2 &= \frac{1}{N} \sum_{\{S\}} \sum_{i(\neq k, k+d)} P(S_i)V(S_k)P(S_k | S_i) \\ &\quad \times V(S_{k+d})P(S_{k+d} | S_i). \end{aligned} \quad (\text{A5})$$

K_1 corresponds to the term $i = k$ (or $k + d$) in (A3) whereas in K_2 , $i \neq k, k + d$. Let us consider K_2 . The summation over $S_i = A$ or B in (A5) leads to

$$\sum_{S_i = A, B} P(S_i)P(S_k | S_i)P(S_{k+d} | S_i) = P(S_k, S_{k+d}). \quad (\text{A6})$$

Here $P(S_k, S_{k+d})$ is the probability (not conditional) that the atom at R_k is in state S_k , and simultaneously the nearest-neighbor atom at R_{k+d} is in state S_{k+d} . One can easily convince oneself that since $P(S_k, S_{k+d})$ must be independent of k , for consistency reasons up to order $O(1/T)$,

$$P(S_k, S_{k+d}) = P(S_k)P(S_{k+d}). \quad (\text{A7})$$

The above can be checked explicitly by using the form (6) and the relation (11) together with the fact that $P(S_k)$ must be independent of k . Therefore

$$NK_2 = [\langle V(S_k) \rangle]^2 = V_0^2. \quad (\text{A8})$$

Since in U_2 the potentials are measured relative to V_0 , after subtraction K_2 does not give any contribution.

Performing the summation over the values of S_k, S_{k+d} in (A4) one can write

$$\begin{aligned} NK_1 &= (V_A - V_B)[V_A c P(A_{k+d} | A_k) \\ &\quad + V_B(1-c)P(A_{k+d} | B_k)] + V_B V_0. \end{aligned} \quad (\text{A9})$$

Here (3) and $P(S_k) = c$ or $(1-c)$ independently of k have been used. In order to proceed we note, that because of (11)

$$cP(A_k | A_i) + (1-c)P(A_k | B_i) = c. \quad (\text{A10})$$

Using this and (6) in (A9), we finally obtain

$$\begin{aligned} NK_1 &= c^2(V_A - V_B)^2 \\ &\quad \times \left[1 - \frac{(1-c)W}{k_B T} \sum_{d_1} [P(A_{k+d+d_1} | A_k) - c] \right] \\ &\quad + V_B [c(V_A - V_B) + V_0], \end{aligned} \quad (\text{A11})$$

where d_1 denotes nearest neighbors of $k + d$. Subtracting V_0^2 from (A11) the terms independent of W cancel. Using then (A2) and (A11) we finally obtain

$$\begin{aligned} U_2 &= c(1-c)(V_A - V_B)^2 \frac{1}{N} \\ &\quad \times \sum_k \delta(r - R_k) \left[\delta(r' - R_k) - \frac{cW}{k_B T} \sum_{d, d_1} \delta(r' - R_k - d) \right. \\ &\quad \left. + [P(A_{k+d+d_1} | A_k) - c] \right]. \end{aligned} \quad (\text{A12})$$

Since we are interested in expressions valid to first order in $1/(k_B T)$ according to (7) it is only the term $d = -d_1$ in (A12) which should be retained. With this one arrives at the result given in the text by (13), $T = T_0$.

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- ¹⁵This is clearly explained in the review paper by B. L. Alt'shuler and A. G. Aronov, in *Electron-Electron Interaction in Disordered Systems*, edited by A. L. Efros and M. Pollack (North-Holland, Amsterdam, 1985).
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