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CPA Study of the Electrical Conductivity for Various Percolation Models

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Transport properties are examined for randomly disordered systems comprising a mixture of conducting and insulating components. The tight-binding models on a s.c. lattice are specialized to purely diagonal disorder, off-diagonal disorder of the multiplicative and additive type, also in the presence of electron–electron interaction; the percolation limits are reached by the breaking of inter- or intra-species links. The effective medium is provided by the CPA (coherent potential approximation) and its extended version ODCPA, if necessary combined with the Hartree-Fock approximation. The dc conductivity σ vanishes at a critical concentration x_c of inaccessible sites at fixed Fermi energy. The ODCPA involving vertex corrections refers to localization in the middle of the band. Numerical $\sigma(x)$-results are presented.

Untersucht werden Transporteigenschaften stochastisch ungeordneter Systeme, die aus einem Gemisch von leitender und isolierender Komponente bestehen. Die tight-binding-Modelle zum s.c.-Gitter sind auf diagonale bzw. nichtdiagonale Unordnung vom multiplikativen und additiven Typ — auch bei Elektron–Elektron-Wechselwirkung — spezialisiert; die Perkolationsfälle werden durch Unterbrechen von Verbindungen zwischen Atomen unterschiedlicher oder gleicher Sorte erreicht. Das effektive Medium wird durch die CPA (kohärente Potentialnäherung) und deren erweiterte Version ODCPA eingeführt, gegebenenfalls kombiniert mit der Hartree-Fock-Näherung. Die statische elektrische Leitfähigkeit σ verschwindet bei fester Fermi-Energie an einer kritischen Konzentration x_c von unzugänglichen Gitterplätzen. Die ODCPA, die Vertexkorrekturen enthält, führt zur Lokalisierung in der Bandmitte. Numerische $\sigma(x)$-Ergebnisse sind dargestellt.

1. Introduction

Both classical and quantum percolation models can be set up in the same manner, e.g. by a random mixture of accessible and inaccessible sites (or bonds) in a lattice (metal–insulator system). However, these random (geometrical) characteristics are not sufficient to describe uniquely the electrical conductivity. Quantum percolation [1, 2] must include in contrast to the classical concept [3, 4] localized electron states (Anderson localization, cf., e.g. [5]).

Usual methods to treat the percolation problem are the numerical analysis of network models [3, 4], computer simulation [1, 2, 6], and renormalization-group technique [7]. As an alternative analytical tool, the effective-medium approach gives a good description of the transport properties of disordered systems except in the critical region, as proved in [3, 4, 7 to 9]. In the alloy context the effective-medium theory is provided by the coherent potential approximation (CPA) [10]. Some types of percolation limits have been discussed within the single-site CPA [11 to 14], also in connection with electron–electron interaction [15], and in the single-bond CPA [16, 17]. However, the CPA fails to give cluster effects and electron localization which are relevant close to the percolation threshold (see [6, 8]). Here a critical-path analysis would be necessary.

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In this paper we compare CPA expressions of the conductivity for several alloy models on an equal footing. The percolation cases are studied without and with chemical constraint. In Section 2 the percolative dc conductivity at $T = 0$ is evaluated analytically in the presence of diagonal as well as off-diagonal disorder of the multiplicative and additive type in the tight-binding Hamiltonian. Electron–electron interaction is taken into account in the Hartree-Fock approximation (Section 3). Numerical results are given in Section 4.

2. CPA Schemes and Conductivities

2.1 Basis of the model calculations

The standard model of A_xB_{1-x} alloys is given by the one-electron tight-binding Hamiltonian (spinless form)

$$H^{\{\nu\}} = \sum_i \varepsilon_i^\nu c_i^+ c_i + \sum_{\substack{ij \\ (i \neq j)}} t_{ij}^{\nu\mu} c_i^+ c_j = H^B + V^{\{\nu\}} \tag{1}$$

within an arbitrary configuration $\{\nu\}$; ν and μ refer to the atomic kind (A or B) on the sites i and j of a simple cubic lattice. The random hopping energies $t_{ij}^{\nu\mu}$ are restricted to nearest neighbour (n.n.) elements $t^{\nu\mu}$. The periodic part H^B is associated with the pure B-crystal. Propose that the random potential is additive, i.e. $V^{\{\nu\}} = \sum_i V_i^\nu$, but the single-site potentials V_i^ν are not necessarily localized on the corresponding sites. Moreover, the case of a quasi-diagonal random operator will be also included.

The configurationally averaged ($\langle ... \rangle$) one-particle Green function can be written as

$$\mathcal{G}(z) = \langle G^{\{\nu\}}(z) \rangle = \left\langle \left[z - H^B - \sum_i V_i^\nu \right]^{-1} \right\rangle = [z - H^B - \Sigma(z)]^{-1} . \tag{2}$$

The coherent potential $\Sigma = \sum_i \Sigma_i$ is determined in the one-centre approximation by the CPA self-consistency condition

$$\langle T_i^\nu(z) \rangle = \langle \left(V_i^\nu - \Sigma_i(z)\right) [1 - \mathcal{G}(z) \left(V_i^\nu - \Sigma_i(z)\right)]^{-1} \rangle = 0 \tag{3}$$

imposed on the single-site scattering operator T_i^ν, where $\langle T_i^\nu \rangle = x T_i^A + (1 - x)\, T_i^B$.

The scalar dc conductivity σ can be found from the Kubo-Greenwood formula (cubic symmetry is presumed)

$$\sigma = -\frac{1}{6\pi\Omega} \int_{-\infty}^{\infty} dE \left(-\frac{\partial f(E)}{\partial E} \right) \langle \mathrm{tr} \{ \left(G^{\{\nu\}}(E^+) - G^{\{\nu\}}(E^-)\right) \boldsymbol{j}^{\{\nu\}} \left(G^{\{\nu\}}(E^+) - G^{\{\nu\}}(E^-)\right) \boldsymbol{j}^{\{\nu\}} \} \rangle , \tag{4}$$

where Ω is the volume of the system, and $E^\pm = E \pm i0$. At $T = 0$ we have $-\partial\left(f(E)\right)/\partial E = \delta(E - E_F)$ with E_F being the Fermi energy. The trace runs over one-particle states (the spin is already taken into account by an extra factor of 2). In Wannier representation the matrix elements of the configuration-dependent current operator read $\boldsymbol{j}_{ij}^{\nu\mu} = -iet_{ij}^{\nu\mu}(\boldsymbol{R}_i - \boldsymbol{R}_j)$, where $\boldsymbol{R}_i$ denotes the position vector of the site i.

The electronic density of states follows from

$$\varrho(E) = -\frac{1}{\pi} \mathrm{Im}\, F(E^+) , \tag{5}$$

where

$$F(z) = \frac{1}{N} \sum_{\boldsymbol{k}} \mathcal{G}_{\boldsymbol{k}}(z) . \tag{6}$$

N is the number of the lattice sites.

The model calculations are based on the customary ansatz [10, 18] for the unperturbed B-band:

$$\varrho^{\mathrm{B}}(E) = \frac{1}{N}\sum_{\boldsymbol{k}} \delta\big(E - t^{\mathrm{BB}} s(\boldsymbol{k})\big) = \frac{2}{\pi w^{\mathrm{B}}}\left[1 - \left(\frac{E}{w^{\mathrm{B}}}\right)^2\right]^{1/2} \theta(w^{\mathrm{B}} - |E|)\,, \tag{7}$$

which implies

$$\frac{1}{N}\sum_{\boldsymbol{k}} \delta\big(E - t^{\mathrm{BB}} s(\boldsymbol{k})\big)\,\big(t^{\mathrm{BB}}\nabla_{\boldsymbol{k}} s(\boldsymbol{k})\big)^2 = \frac{2(v_{\mathrm{m}}^{\mathrm{B}})^2}{\pi w^{\mathrm{B}}}\left[1 - \left(\frac{E}{w^{\mathrm{B}}}\right)^2\right]^{3/2} \theta(w^{\mathrm{B}} - |E|)\,. \tag{8}$$

Thereby, $\boldsymbol{k}$-summations can be performed analytically. Here $s(\boldsymbol{k}) = \sum_{j(\neq i:\,\mathrm{u.n.})} \mathrm{e}^{i\boldsymbol{k}(\boldsymbol{R}_j - \boldsymbol{R}_i)}$, $\varepsilon^{\mathrm{B}} = 0$, $w^{\mathrm{B}} = 6t^{\mathrm{BB}}$ is the half-bandwidth, and $v_{\mathrm{m}}^{\mathrm{B}} = \big(a/\sqrt{3}\big)\, w^{\mathrm{B}}$ denotes the maximum velocity in the B-band expressed by the lattice constant a.

2.2 Site randomness (SR)

In the random site model there is only diagonal disorder in (1) subject to the probability distribution

$$P(\varepsilon_i') = x\,\delta(\varepsilon_i' - \varepsilon^{\mathrm{A}}) + (1 - x)\,\delta(\varepsilon_i')\,. \tag{9}$$

This means $\langle \ldots \rangle = \int \mathrm{d}\varepsilon_i'\, P(\varepsilon_i') \ldots$. Consider the strong scattering situation (split-band case) with $\varepsilon^{\mathrm{A}} \gg w^{\mathrm{B}}$. In the following we put $w^{\mathrm{B}} = 1$. Then the self-energy resulting from (3) satisfies the equation

$$\Sigma(z) = \frac{x\varepsilon^{\mathrm{A}}}{1 - \big(\varepsilon^{\mathrm{A}} - \Sigma(z)\big)\, F(z)}, \tag{10}$$

where, according to (6) and (7), $F(z)$ takes the form

$$F(z) = 2\Big(z - \Sigma(z) - \sqrt{\big(z - \Sigma(z)\big)^2 - 1}\Big). \tag{11}$$

Concerning the conductivity (4) no vertex corrections occur in the presence of SR [10] so that

$$\sigma = \frac{2e^2}{3\pi\Omega}\sum_{\boldsymbol{k}} \big(\operatorname{Im} \mathcal{G}_{\boldsymbol{k}}(E_{\mathrm{F}}^+)\big)^2\,\big(t^{\mathrm{BB}}\nabla_{\boldsymbol{k}} s(\boldsymbol{k})\big)^2\,, \tag{12}$$

which leads via (8) to [19]

$$\sigma = 2\sigma_0\left[2\,\big(\operatorname{Im}\Sigma(E_{\mathrm{F}}^+)\big)^2 + \frac{1}{\operatorname{Im}\Sigma(E_{\mathrm{F}}^+)}\operatorname{Re}\big\{i\sqrt{1-\hat{z}^2}\big(i(1-\hat{z}^2) + 3\hat{z}\operatorname{Im}\Sigma(E_{\mathrm{F}}^+)\big)\big\}\right], \tag{13}$$

where $\hat{z} = E_{\mathrm{F}}^+ - \Sigma(E_{\mathrm{F}}^+)$ and

$$\sigma_0 = \frac{e^2 (v_{\mathrm{m}}^{\mathrm{B}})^2\, N}{3\pi\Omega}. \tag{14}$$

More explicitly, (13) can be rewritten as

$$\sigma = \sigma_0\,\big(\operatorname{Im} F(E_{\mathrm{F}}^+)\big)^2\,\big(\tfrac{1}{2} + [1 - \tfrac{1}{4}\,|F(E_{\mathrm{F}}^+)|^2]^{-1}\big) \tag{15a}$$

or [20]

$$\sigma = \sigma_0 \pi^2 \varrho^2(E_{\mathrm{F}})\left(\frac{3}{2} + \frac{\pi\varrho(E_{\mathrm{F}})}{4\,|\operatorname{Im}\Sigma(E_{\mathrm{F}}^+)|}\right). \tag{15b}$$

The site percolation model is obtained by putting an infinite potential on A-sites (lattice gas model [14]). In the limit $\varepsilon^{\mathrm{A}} \to \infty$ simple relations arise from (10), (11), and (15):

$$\Sigma(z) = -\frac{x}{F(z)}, \tag{16}$$

$$F(z) = 2\left(z - \sqrt{z^2 - 1 + x}\right) = 2\left(z - \sqrt{x - x_{\mathrm{c}}(z)}\right), \tag{17}$$

$$x_{\mathrm{c}}(z) = 1 - z^2, \tag{18}$$

$$\sigma = 2\sigma_0\left(x_{\mathrm{c}}(E_{\mathrm{F}}) - x\right)\left(1 + \frac{2}{x}\right)\theta\left(x_{\mathrm{c}}(E_{\mathrm{F}}) - x\right). \tag{19}$$

The real value $x_{\mathrm{c}}(E_{\mathrm{F}})$ can be understood as a critical concentration for the transition from the conducting to the insulating region. Here, at fixed E_{F}, x_{c} is immediately connected with the band edge. However, x_{c} does not represent a true percolation threshold between extended and localized states (in the sense of a mobility edge). Note that the result (19) yields σ explicitly without further CPA procedure. Expression (19) was found in a different way in [12] by using a 2×2 matrix formalism (cf., e.g. [13]).

2.3 Multiplicative random hopping (MRH)

The off-diagonal randomness in (1) is chosen to be of the form $t^{\mathrm{AB}} = \sqrt{t^{\mathrm{AA}} t^{\mathrm{BB}}}$. This condition is fulfilled if

$$t_{ij}^{\nu\mu} = \zeta_i^{\nu} t^{\mathrm{BB}} \zeta_j^{\mu}, \qquad (i, j: \text{n.n.}). \tag{20}$$

Now it holds $w^{\nu} = 6t^{\mathrm{BB}}\zeta^{\nu}$ for the half-bandwidth of the pure ν-component. In order to compare the results, $w^{\mathrm{B}} = 1$ is retained. The random parameters ζ_i^{ν} give rise to the extension of the distribution (9) as

$$P(\varepsilon_i^{\nu}, \zeta_i^{\nu}) = x\,\delta(\varepsilon_i^{\nu} - \varepsilon^{\mathrm{A}})\,\delta(\zeta_i^{\nu} - \zeta^{\mathrm{A}}) + (1 - x)\,\delta(\varepsilon_i^{\nu})\,\delta(\zeta_i^{\nu} - 1). \tag{21}$$

Let us transform the Hamiltonian (1) and consequently the Green function through [21, 22]

$$\tilde{H}^{\{\nu\}} = \zeta^{\{\nu\}-1} H^{\{\nu\}} \zeta^{\{\nu\}-1}, \tag{22}$$

$$\tilde{G}^{\{\nu\}}(z) = \zeta^{\{\nu\}} G^{\{\nu\}}(z)\,\zeta^{\{\nu\}}, \tag{23}$$

where $\zeta^{\{\nu\}}$ is a non-singular ($\zeta^{\mathrm{A}}\zeta^{\mathrm{B}} \neq 0$), diagonal operator defined by $\zeta^{\{\nu\}} = \sum_i \zeta_i^{\nu} c_i^{+} c_i$. The new $\tilde{H}^{\{\nu\}}$ has no off-diagonal disorder so that standard CPA technique can be applied. In other words, $H^{\{\nu\}}$ itself is a so-called quasi-diagonal operator under the requirement (20). In analogy to (2) and (3), the renormalized averaged Greenian $\tilde{\mathcal{G}}(z)$ and coherent potential $\tilde{\Sigma}(z)$ are determined by

$$\tilde{\mathcal{G}}(z) = \langle \tilde{G}^{\{\nu\}}(z) \rangle = \langle [\zeta^{\{\nu\}-1}\left(z - \sum_i V_i^{\nu}\right)\zeta^{\{\nu\}-1} - H^{\mathrm{B}}]^{-1} \rangle = \left(\tilde{\Sigma}(z) - H^{\mathrm{B}}\right)^{-1}, \tag{24}$$

$$\tilde{\Sigma}(z) + x\frac{\varepsilon^{\mathrm{A}} - z}{\zeta^{\mathrm{A}2}} - (1 - x)\,z - \left(\tilde{\Sigma}(z) - z\right)\left(\tilde{\Sigma}(z) + \frac{\varepsilon^{\mathrm{A}} - z}{\zeta^{\mathrm{A}2}}\right)\tilde{F}(z) = 0, \tag{25}$$

where

$$\tilde{F}(z) = \frac{1}{N}\sum_k \tilde{\mathcal{G}}\ (z) = 2\left(\tilde{\Sigma}(z) - \sqrt{(\tilde{\Sigma}(z))^2 - 1}\right). \tag{26}$$

Here $\tilde{\mathcal{G}}_{\boldsymbol{k}}(z) = \left(\tilde{\Sigma}(z) - t^{\mathrm{BB}} s(\boldsymbol{k})\right)^{-1}$ and (7) were used. By performing the transformation (23) in (4) the original random current operator goes over in a configuration-independent one. Hence, the σ-formula takes the same form as (12) but with $\tilde{\mathcal{G}}$ instead of $\mathcal{G}$. In view of (15a) the conductivity reads [21, 22]

$$\sigma = \sigma_0 (\mathrm{Im}\, \tilde{F}(E_{\mathrm{F}}^+))^2 \left(\tfrac{1}{2} + [1 - \tfrac{1}{4} |\tilde{F}(E_{\mathrm{F}}^+)|^2]^{-1}\right) . \tag{27}$$

Note that the form (15b) is impossible in this scheme.

In the limit of zero A-bandwidth, MRH causes simultaneously $t^{\mathrm{AA}} = t^{\mathrm{AB}} = 0$, thus permitting electron hopping between n.n. B-atoms only (percolation model). From (25) one gets for $\zeta^{\mathrm{A2}} \to 0$

$$\tilde{\Sigma}(z) = z + \frac{x}{\tilde{F}(z)} \tag{28}$$

provided that $z \neq \varepsilon^{\mathrm{A}}$. Then $\tilde{F}(z)$ coincides exactly with $F(z)$ in (17). Therefore, in the limit $w^{\mathrm{A}} \to 0$ we find for σ the expression (19).

To calculate the density of states in the case of MRH one must return to the unrenormalized propagator $F(z)$. Introduce the partial density of states $\varrho^{\nu}(E) = -\frac{1}{\pi} \mathrm{Im}\, G_{ii}^{\nu}(E^+)$ in terms of the conditionally averaged propagator

$$G_{ii}^{\nu}(z) = \frac{1}{\zeta^{\nu 2}} \left[\tilde{F}^{-1}(z) + \frac{z - \varepsilon^{\nu}}{\zeta^{\nu 2}} - \tilde{\Sigma}(z)\right]^{-1} , \tag{29}$$

where the inverse transformation of (23) as well as (24), (26), and $F(z) = \langle G_{ii}^{\nu}(z) \rangle$ have been employed. Now we carry out the percolation limit $\zeta^{\mathrm{A2}} \to 0$ to get

$$\varrho(E) = x\, \delta(E - \varepsilon^{\mathrm{A}}) + \frac{2}{\pi} \sqrt{x_{\mathrm{c}}(E) - x} \tag{30}$$

being valid for $x < x_{\mathrm{c}}$.

With respect to the critical concentration and the conductivity in the percolation limits no difference appears between the SR and MRH (for $E_{\mathrm{F}} \neq \varepsilon^{\mathrm{A}}$) models. This represents just the independent band limit.

2.4 Additive random hopping (ARH)

Another type of off-diagonal disorder arises from the assumption $t^{\mathrm{AB}} = \frac{1}{2} (t^{\mathrm{AA}} + t^{\mathrm{BB}})$, that means

$$t_{ij}^{\nu\mu} = t^{\mathrm{BB}} + t_i^{\nu} + t_j^{\mu} , \qquad (i, j\colon \text{n.n.}) . \tag{31}$$

Here the percolation limit $t^{\mathrm{AA}} = 0$ can be chosen a priori, and we are left with

$$P(t_i^{\nu}) = x\, \delta\left(t_i^{\nu} + \tfrac{1}{2} t^{\mathrm{BB}}\right) + (1 - x)\, \delta(t_i^{\nu}) . \tag{32}$$

There are three possibilities for the electron transfer between n.n. atoms: accessible (B–B), semi-accessible (A–B), and blocked (A–A). Moreover, by setting $\varepsilon^{\mathrm{A}} = 0$ this model possesses bond-type character. As a consequence of (2) with a finite-range V_i^{ν}, the averaged Green function

$$\mathcal{G}_{\boldsymbol{k}}(z) = [z - t^{\mathrm{BB}} s(\boldsymbol{k}) - \Sigma(\boldsymbol{k}, z)]^{-1} \tag{33}$$

involves the momentum-dependent self-energy

$$\Sigma(\boldsymbol{k}, z) = \Sigma_0(z) + 2\Sigma_1(z)\, s(\boldsymbol{k}) + \Sigma_2(z)\, s^2(\boldsymbol{k}) , \tag{34}$$

where Σ_0, Σ_1, and Σ_2 result from the coupled self-consistency equations $\langle \tau_{ii}^{\nu}(z) \rangle = 0$ ($l = 0, 1, 2$) [23] originated from (3).

The conductivity formula (4) takes now the form

$$\sigma = \frac{1}{6\pi\Omega}\left[2\Pi(E_{\mathrm{F}}^{+}, E_{\mathrm{F}}^{-}) - \Pi(E_{\mathrm{F}}^{+}, E_{\mathrm{F}}^{+}) - \Pi(E_{\mathrm{F}}^{-}, E_{\mathrm{F}}^{-})\right], \tag{35}$$

where $\Pi(z, z') = \langle \mathrm{tr}\,\{G^{\{\nu\}}(z)\,\boldsymbol{j}^{\{\nu\}}G^{\{\nu\}}(z')\,\boldsymbol{j}^{\{\nu\}}\}\rangle$ cannot be factorized into a product of mean values. However, one finds analytically [18, 23] the solution

$$\Pi(z, z') = e^2 \sum_{\boldsymbol{k}} \{\mathscr{G}_{\boldsymbol{k}}(z)\,\mathscr{G}_{\boldsymbol{k}}(z')\,[\nabla_{\boldsymbol{k}}(t^{\mathrm{BB}}s(\boldsymbol{k}) + \tfrac{1}{2}\,(\Sigma(\boldsymbol{k}, z) + \Sigma(\boldsymbol{k}, z')))]^2 +$$
$$+ \left(\Sigma_2(z)\,\mathscr{G}_{\boldsymbol{k}}(z') + \Sigma_2(z')\,\mathscr{G}_{\boldsymbol{k}}(z)\right)[\nabla_{\boldsymbol{k}}s(\boldsymbol{k})]^2\} \tag{36}$$

involving vertex corrections. These vertex corrections are caused by the fluctuating current operator $\boldsymbol{j}^{\{\nu\}} = \boldsymbol{j}^{\mathrm{B}} + \boldsymbol{j}^{(1)\{\nu\}}$. An analogous calculation with the periodic current $\langle \boldsymbol{j}^{\{\nu\}}\rangle_{\boldsymbol{k}} = e(1-x)\,t^{\mathrm{BB}}\nabla_{\boldsymbol{k}}s(\boldsymbol{k})$ instead of $\boldsymbol{j}^{\{\nu\}}$ would lead to ($w^{\mathrm{B}} = 1$ as before)

$$\sigma[\boldsymbol{j}^{\mathrm{B}} + \langle \boldsymbol{j}^{(1)\{\nu\}}\rangle] = (1-x)^2\,\sigma[\boldsymbol{j}^{\mathrm{B}}], \tag{37}$$

where $\sigma[\boldsymbol{j}^{\mathrm{B}}]$ is defined by (35) setting $\Sigma_1 = \Sigma_2 = 0$ in (36) but not in (34). The quantity $\sigma[\boldsymbol{j}^{\mathrm{B}} + \boldsymbol{j}^{(1)\{\nu\}}] - \sigma[\boldsymbol{j}^{\mathrm{B}} + \langle \boldsymbol{j}^{(1)\{\nu\}}\rangle]$ is a measure for the statistical correlations (vertex corrections). Indeed, the ARH model is an alternative of the "site" percolation models in Sections 2.2 and 2.3.

The actual σ-calculation requires the $\boldsymbol{k}$-summation in (36) on the basis of (8). This has been done in [18] by the residue method.

3. Percolation Limit in the Presence of Electron–Electron Interaction

Let us add a random Hubbard term

$$H_U^{\{\nu\}} = \tfrac{1}{2}\sum_{i\sigma} U_i^{\nu} n_{i\sigma} n_{i-\sigma}, \qquad n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma} \tag{38}$$

to (1) (with spin included). Treating (38) in the Hartree-Fock approximation one can reduce the total Hamiltonian to the one-particle form with spin-dependent site energies $\varepsilon_{i\sigma}^{\nu} = \varepsilon_i^{\nu} + U_i^{\nu} n_{i-\sigma}^{\nu}$, the probability distribution of which reads

$$P(\varepsilon_{i\sigma}^{\nu}) = x\,\delta(\varepsilon_{i\sigma}^{\nu} - \varepsilon^{\mathrm{A}} - U^{\mathrm{A}} n_{-\sigma}^{\mathrm{A}}) + (1-x)\,\delta(\varepsilon_{i\sigma}^{\nu} - U^{\mathrm{B}} n_{-\sigma}^{\mathrm{B}}). \tag{39}$$

As in (21) or by combination with (32), one can incorporate the cases of MRH or ARH, respectively.

The present spin-dependent problem can be embedded into the CPA scheme outlined in Section 2.1. The mean number of electrons with spin σ at ν sites is determined self-consistently by

$$n_{i\sigma}^{\nu} = -\frac{1}{\pi}\int_{-\infty}^{E_{\mathrm{F}}} \mathrm{d}E\ \mathrm{Im}\, G_{ii\sigma}^{\nu}(E^{+}) \equiv n_{\sigma}^{\nu}, \tag{40}$$

where

$$G_{ii\sigma}^{\nu}(z) = \left(\mathscr{G}_{\sigma}(z) + \mathscr{G}_{\sigma}(z)\,T_{i\sigma}^{\nu}(z)\,\mathscr{G}_{\sigma}(z)\right)_{ii}. \tag{41}$$

The explicit expressions for the partially averaged local Green function are $G_{ii\sigma}^{\nu}(z) = F_{\sigma}(z)\left(1 - (\varepsilon_{i\sigma}^{\nu} - \Sigma_{\sigma}(z))\,F_{\sigma}(z)\right)^{-1}$ (SR), available from (29) (MRH), and given in [23] (ARH). At given n (mean number of electrons per site) the Fermi energy obeys the equation

$$n = \sum_{\sigma} n_{\sigma} = -\frac{1}{\pi}\sum_{\sigma}\int_{-\infty}^{E_{\mathrm{F}}} \mathrm{d}E\ \mathrm{Im}\, F_{\sigma}(E^{+}). \tag{42}$$

Moreover, the σ-formulae (12) to (15), (19), (27), and (35) to (37) remain valid but instead of the factor 2 we have to write $\sigma = \sum_{\sigma} \sigma_{\sigma}$, where σ_{σ} is defined with the corresponding spin-dependent quantities.

In the percolation limit $\zeta^{A2} \to 0$ ($z \doteq \varepsilon_{\sigma}^{A}$, $w^{B} = 1$) of the MRH model the scheme given in Section 2.3 can be formulated for each spin direction as follows:

$$\tilde{\Sigma}_{\sigma}(z) = z - \varepsilon_{\sigma}^{B} + \frac{x}{\tilde{F}_{\sigma}(z)}, \tag{43}$$

$$\tilde{F}_{\sigma}(z) = 2\left(z - \varepsilon_{\sigma}^{B} - \sqrt{x - x_{c\sigma}(z)}\right), \tag{44}$$

$$x_{c\sigma}(z) = 1 - (z - \varepsilon_{\sigma}^{B})^{2}, \tag{45}$$

$$\sigma_{\sigma} = \sigma_{0}\left(x_{c\sigma}(E_{F}) - x\right)\left(1 + \frac{2}{x}\right)\theta\left(x_{c\sigma}(E_{F}) - x\right), \tag{46}$$

$$\varrho_{\sigma}^{B}(E) = \frac{2}{\pi(1-x)}\sqrt{x_{c\sigma}(E) - x}, \tag{47}$$

and $\varrho_{\sigma}^{A}(E) = \delta(E - \varepsilon_{\sigma}^{A})$. The SR model yields in the limit $\varepsilon^{A} \to \infty$ the same σ-result as (46). Note that relations, which are equivalent to (44) and (47), have been found in [15] for diagonal disorder. By inserting (47) into (40) one obtains

$$n_{\sigma}^{B} = \frac{E_{F} - \varepsilon_{\sigma}^{B}}{\pi(1-x)}\sqrt{x_{c\sigma}(E_{F}) - x} + \frac{1}{\pi}\arcsin\frac{E_{F} - \varepsilon_{\sigma}^{B}}{\sqrt{1-x}} + \frac{1}{2} \tag{48}$$

for $x \leqq x_{c\sigma}(E_{F})$; it holds $n_{\sigma}^{B} = 1$ at $x = x_{c\sigma}(E_{F})$.

It follows a remark on the critical behaviour. In analogy to the usual definition of the scaling law for the conductivity let us write

$$\sigma(x) \propto (x_{c} - x)^{r}, \tag{49}$$

where σ is nonzero for $x < x_{c}$. In view of (19) (or (46)) one deduces $\sigma \propto \left(1 + (2/x_{c})\right) \times$ $\times (x_{c} - x) + (2/x_{c}^{2})(x_{c} - x)^{2} + \ldots$, giving rise to the exponent $r = 1$ from the leading term. Such a critical exponent occurs in other mean field theories [5], too. Note that the exponent associated with the density of extended states takes the value 1/2 according to (17) (cf. also (30) and (47)).

4. Numerical Results and Discussion

The next step is to give some numerical examples for the dc conductivity at several, especially extreme, degrees of disorder. Differences of the various CPA approaches and their percolation limits are illustrated.

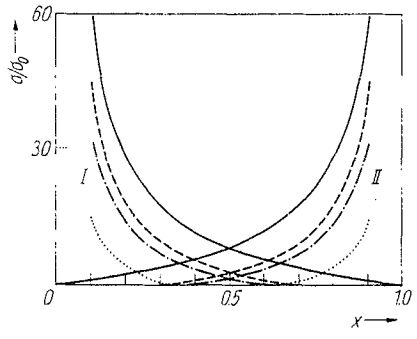

Fig. 1. Conductivity σ (in units of σ_{0}) versus concentration x of A atoms in the SR model with the parameters $\{\varepsilon^{A}, \varepsilon^{B}, w^{A}, w^{B}\} = \{5, 0, 1, 1\}$. Fermi energy $E_{F}\,(\mathrm{I/II}) = 2.5 \mp \tilde{E}_{F}$; $\tilde{E}_{F} = 2.5$ (———), 3.1 (– – – –), 1.9 (—·—·—), 1.7 (· · · · · ·)

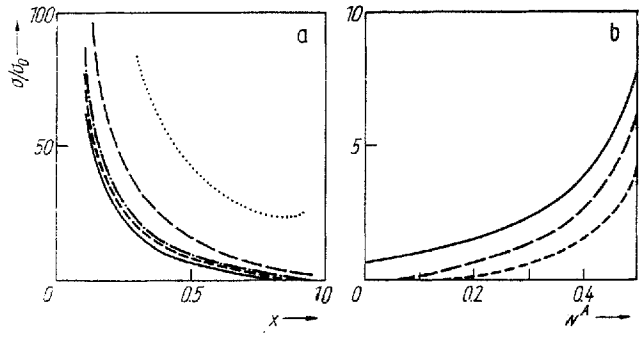

Fig. 2. Conductivity σ as a function of the concentration x and the half-bandwidth w^A of the A component in the ARH model for $\{\varepsilon^A, \varepsilon^B, w^B, E_F\} = \{0, 0, 1, 0.5\}$. a) $w^A = 0$ (———), 0.15 (– – – –), 0.2 (—·—·—), 0.4 (— — —), 0.6 (· · · · ·); b) $x = 0.8$ (———), 0.85 (— — —), 0.9 (– – – –)

Fig. 1 shows the variation of the conductivity σ (scaled by σ_0 (14)) with the concentration x of A atoms in the split-band case of the SR model. According to the location of the Fermi energy E_F either the B (case I) or the A (II) component is conducting. At a concentration threshold x_c, σ becomes zero because E_F passes the band edge (band edge critical point [5]). If E_F drops in the band centre the values $x_c = 0$ or 1

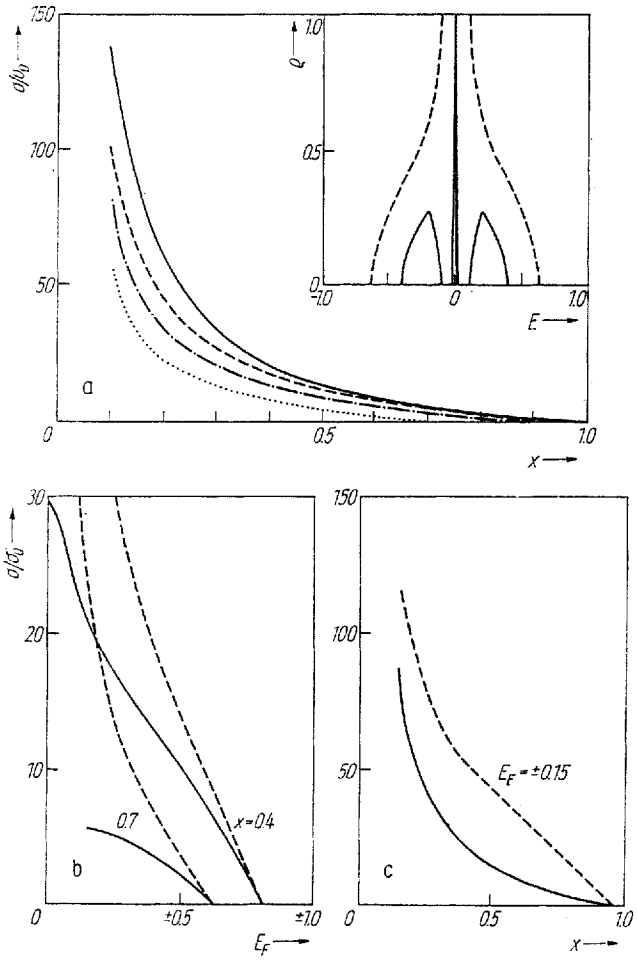

Fig. 3. Conductivity σ in dependence on the Fermi energy E_F and the concentration x of A atoms in the ARH model at $\{\varepsilon^A, \varepsilon^B, w^A, w^B\} = \{0, 0, 0, 1\}$. a) σ for $E_F = \pm 0.15$ (———), ± 0.25 (– – – –), ± 0.4 (—·—·—), ± 0.6 (· · · · · ·) compared with the density of states ϱ at $x = 0.7$ (– – – –), 0.95 (———); b) and c) σ with (———) and without (– – – –) vertex corrections

are reached only asymptotically (cf. [16]). A critical exponent, which can be defined here only formally, is found roughly as $r = 1.1 \pm 0.2$ being nearly independent of E_F. Note that $r = 1.5 \pm 0.2$ results from the classical network calculation [4] for the site model.

Fig. 2 exhibits the onset of a conductivity threshold $\sigma(x_c) = 0$ in dependence on the half-bandwidth w^A and the concentration x of the A component for the ARH model. If the A sites become more accessible ($w^A > 0.2$ at fixed E_F here) the threshold vanishes. One sees a continuous transition of the σ-curves (Fig. 2a) from small to zero w^A, i.e. from the alloy to the percolation limit.

In Fig. 3 σ-results are presented for the ARH model in the percolation limit $t^{AA} = 0$. The critical exponent is obtained from Fig. 3a as $r = 1.05 \pm 0.15$. Vertex corrections plotted in Fig. 3b and c strongly diminish the conductivity, whereas the effective band edges and the critical concentration x_c are not affected. As can be seen from the derivative of σ at x_c in Fig. 3c, the statistical correlations have a marked influence on the critical behaviour. The value $x_c = 0.95$ for $E_F = 0.15$ can be understood as a percolation threshold since the band splits off at this concentration (Fig. 3a). Here a δ-peak appears in the band centre which refers to localized states at A atoms.

Fig. 4 gives a comparison of the σ-results based on the SR, MRH, and ARH models, i.e. in the presence of diagonal disorder, purely off-diagonal disorder of the multiplicative and additive type, respectively. The numerical analysis shows that the CPA results of σ tend continuously to the analytic solution (19) for $w^A \to 0$ at MRH (Fig. 4a) and for $\varepsilon^A \to \infty$ at SR (Fig. 4b). Thus the simple formula (19) seems to be a useful approximation for conductivity estimations. Owing to the "semi-bonds" t^{AB} in the ARH case, higher x values are needed to suppress the conduction. A crossing, obtained in [16] for the conductivities of the site and bond percolation models, cannot be found here between the σ-curves at SR and ARH.

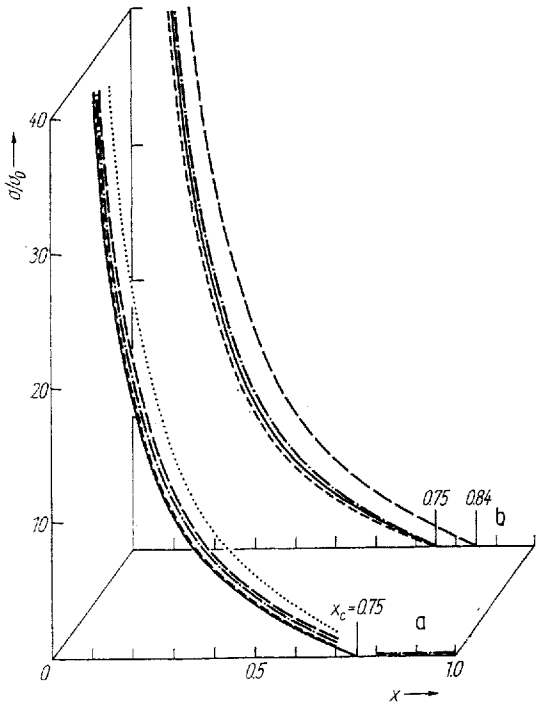

Fig. 4. Conductivity σ plotted against the concentration x of A atoms for the set $\{\varepsilon^B, w^B, E_F\} = \{0, 1, \pm 0.5\}$. Analytical σ-solution (19) (———) compared with numerical results of a) MRH for $\varepsilon^A = 0$, $w^A = 0.01$ (– – – –), 0.05 (— · — · —), 0.1 (— — —), 0.2 (· · · · ·); b) SR for $\varepsilon^A = 10$, $w^A = 1$ at $E_F = 0.5$ (– – – –), -0.5 (— · — · —), and ARH (— — —) for $\varepsilon^A = w^A = 0$

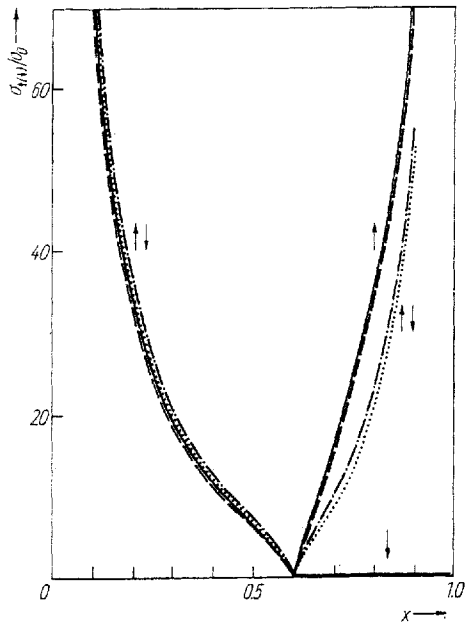

Fig. 5. Spin-dependent conductivity $\sigma_{\uparrow(\downarrow)}$ (scaled by σ_0) versus concentration x of A atoms in the SR case for $\{\varepsilon^A, \varepsilon^B, w^A, w^B, U^B, n\} = \{0.6, 0, 0.6, 0.6, 0, 0.8\}$ at various interaction strengths $U^A = 0$ (—·—·—), 0.5 (· · · · · ·), 1.5 (———), 2.5 (— — —)

The $\sigma_{\uparrow(\downarrow)}(x)$-plot in Fig. 5 shows some form of spin polarization by varying the Coulomb repulsion U^A. The calculation is based on the Hartree-Fock CPA treatment for a Wolff model ($U^B = 0$) alloy. In the paramagnetic case σ_σ vanishes at $x = 0.6$. There saturated ferromagnetic solutions occur with increasing U^A-values.

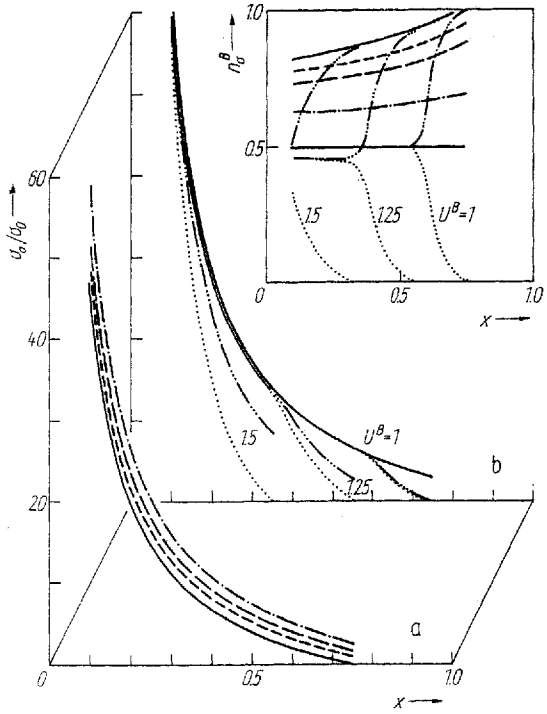

Fig. 6. Spin-dependent conductivity σ_σ and mean number of electrons n_σ^B — based on the solutions (46) and (48), respectively — in dependence on the concentration x of inaccessible A sites and the Coulomb repulsion U^B for the set $\{\varepsilon^A, \varepsilon^B, w^A, w^B, U^A, E_F\} = \{0, 0, 0, 1, 0, 0.5\}$. a) $\sigma_\uparrow = \sigma_\downarrow$ for $U^B = 0$ (———), 0.1 (— — —), 0.2 (— — —), 0.5 (—·—·—); b) $\sigma_\uparrow = \sigma_\downarrow$ (———) and $\sigma_\uparrow$ (—·····—), $\sigma_\downarrow$ (· · · · · ·); n_σ^B-curves are distinguished as in a) and b)

The results (46) and (48) of the spin-correlated percolation model are shown in Fig. 6. The $\sigma_\sigma(x)$-curves for small U^B (Fig. 6a) refer to the continuity to the uncorrelated case (19). The onset of ferromagnetism (Fig. 6b and for n_σ^B) fulfils a Stoner criterion estimated by $U^B(1-x)^{-1/2} > \pi/2$. This is a modification of the corresponding inequality in [15]. For $U^B = 1$ the para- and ferromagnetic solutions are given; here in the ferromagnetic case $\sigma_\uparrow$ is equal to $\sigma_\downarrow$ due to a symmetric spin-band filling (particle-hole symmetry).

To conclude: having adopted the CPA to the conductivity σ of A_xB_{1-x} alloys one can treat the breaking of links in the lattice model coming from the extended-state side of the problem. Although the common CPA yields no band tailing, this perturbative method can be used to deal with the extended states within the band. Thus σ vanishes at a critical concentration x_c of the inaccessible component but the scaling law cannot predicted exactly. In case that only diagonal or multiplicative off-diagonal disorder are considered the theory does not involve statistical correlations. However, a more realistic situation is achieved if the ODCPA introduces nonvanishing vertex corrections to the conductivity. There is some indication of a "true" percolation threshold.

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