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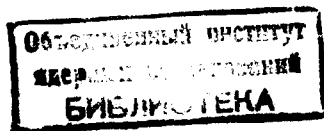# ALLOYS IN OFF-DIAGONAL CPA

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1. Introduction

As has been proved by applying the coherent potential approximation (CPA) and its generalizations to Kubo's current-current correlation function formula, the electrical conductivity of random alloys depends strongly on the type of disorder. Numerical CPA results of the conductivity have been given for diagonal randomness[1-7] and for off-diagonal randomness provided that the transfer integrals are multiplicatively[8-10] (Shiba's condition) or additively[11] dependent on the configurations at the sites linked. For diagonal disorder at finite temperature, the effect of electron-phonon interaction on the dc conductivity was investigated by Chen et al.[12] (see also [13]), and the strain effect was included in [14].

This paper is concerned, on the basis of the theory developed in[15], with the calculation of the temperature-dependent dc con-

ductivity of random off-diagonal alloys in the additive limit. The theoretical background [15] can be summarized as follows. Start with the Kubo-Greenwood formula for the dc-conductivity tensor

$$\sigma_{\alpha\beta} = \frac{1}{2\pi V} \int_{-\infty}^{\infty} d\eta \left(-\frac{\partial f}{\partial \eta}\right) \ll \text{tr}\{G(\eta^+)j_\alpha G(\eta^-)j_\beta + G(\eta^-)j_\alpha G(\eta^+)j_\beta -$$

$$(1.1)$$

$$- G(\eta^+)j_\alpha G(\eta^+)j_\beta - G(\eta^-)j_\alpha G(\eta^-)j_\beta\} >_\theta >_c \ ,$$

where

$$f(\eta) = (I + \exp\{(\eta - \mu)/k_B T\})^{-1} \qquad (1.2)$$

is the Fermi distribution function, V is the volume of the system, μ is the chemical potential, and $\eta^\pm = \eta \pm i0$. In the Wannier space, the Fourier transform $G_{nm}(z;\theta)$ of the one-electron Green function obeys the equation of motion

$$(z - \epsilon^B - E_n)G_{nm}(z;\theta) - \sum_{k(\neq n)}' (h^{BB} + h_n + h_k)G_{km}(z;\theta) =$$

$$(1.3)$$

$$= \delta_{nm} + \theta_n G_{nm}(z;\theta) + \sum_{k(\neq n)}' (\bar\theta_n + \bar\theta_k) G_{km}(z;\theta);$$

and the α-component of the one-electron current operator is given by

$$j_\alpha = j_\alpha^{(0)} + j_\alpha^{(1)} \ , \qquad (1.4)$$

with

$$j_\alpha^{(0)} = -ieh^{BB}\sum_n \sum_{m(\neq n)}' (R_{\alpha n} - R_{\alpha m})a_n^+ a_m, \qquad (1.5)$$

$$j_\alpha^{(1)} = -ie\sum_n \sum_{m(\neq n)}' (h_n + \bar\theta_n)(R_{\alpha n} - R_{\alpha m})(a_n^+ a_m - a_m^+ a_n), (1.6)$$

where $\vec{R}_n$ denotes the position vector of site n in the static lattice, and the prime indicates that only the nearest neighbours are included in the summation. This description is based on the general model Hamiltonian derived in the Appendix. For the additive type of the off-diagonal disorder, the configuration-dependent quantities $[E_n, h_n; \theta_n, \bar\theta_n]$ are equal to $[\epsilon^A - \epsilon^B, \frac{1}{2}(h^{AA} - h^{BB}); \theta^A, \bar\theta^A]$ or $[0, 0; \theta^B, \bar\theta^B]$ according to whether an A or B atom occupies the n-th site, respectively. In generalized alloy analogy, the electron-phonon interaction is described by c-numbers θ_n and $\bar\theta_n$ which fluctuate thermally according to certain Gaussian distributions. The static (adiabatic) approximation is used in order to perform the phonon averaging $<...>_\theta$ and the configuration averaging $<...>_c$ successively (the indices are dropped in the following). After averaging within a modified CPA the correlation function related to $\sigma_{\alpha\alpha}$ was found [15] in $\vec{k}$-space as (cf. [16] in the phononless case)

$$\ll \text{tr}\{G(z_1)j_\alpha G(z_2)j_\alpha\} \gg =$$

$$= e^2 \sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[\frac{\partial}{\partial k_\alpha}\{h^{BB}s(\vec{k}) + \frac{1}{2}(\Sigma(\vec{k},z_1) + \Sigma(\vec{k},z_2))\}]^2 +$$

$$+ e^2 \sum_{\vec{k}} [\sigma_2(z_1)\mathcal{G}_{\vec{k}}(z_2) + \sigma_2(z_2)\mathcal{G}_{\vec{k}}(z_1)](\frac{\partial s(\vec{k})}{\partial k_\alpha})^2 \ , \qquad (1.7)$$

where

$$\mathcal{G}_{\vec{k}}(z) = \ll G(z;\theta) \gg = (z - \epsilon^B - h^{BB}s(\vec{k}) - \Sigma(\vec{k},z))^{-1} \quad (1.8)$$

$$\Sigma(\vec{k}, z) = \sigma_0(z) + 2\sigma_1(z)s(\vec{k}) + \sigma_2(z)s^2(\vec{k}), \quad (1.9)$$

$$s(\vec{k}) = \sum_{m(\neq n)}' e^{i\vec{k}(\vec{R}_m - \vec{R}_n)}. \quad (1.10)$$

These equations are analysed in two steps. Assuming Velický's [1] model for the unperturbed band we analytically perform the $\vec{k}$-space integrations in (1.7) using the residue method (Section 2). The self-energy contributions $\sigma_0, \sigma_1, \sigma_2$ will be determined by solving the CPA self-consistency condition $\ll T_n \gg = 0$ [1]. Numerical results in Section 3 show especially the effect of the vertex corrections included in (1.7).

2. Analytical Evaluation of the Conductivity

To carry out the $\vec{k}$-summation in (1.7) we assume a simple cubic lattice. The quantities describing the unperturbed lattice are approximated by simplified analytic expressions [1] . The density of states of the pure B-band is chosen as

$$\rho^B(E) = \frac{1}{N}\sum_{\vec{k}} \delta(E - \epsilon^B(\vec{k})) = \begin{cases} \frac{2}{\pi}(1 - E^2)^{1/2} & \text{if } |E| \le 1, \\ \\ 0 & \text{otherwise}, \end{cases} \quad (2.1)$$

and, analogously, the mean-square velocity over a constant-energy surface is replaced by

$$(v^B(E))^2 \rho^B(E) =$$
$$= \frac{1}{N}\sum_{\vec{k}}\left[\frac{\partial\epsilon^B(\vec{k})}{\partial\vec{k}}\right]^2 \delta(E - \epsilon^B(\vec{k})) = \begin{cases} \frac{2(v_m^B)^2}{\pi}(1 - E^2)^{3/2} & \text{if } |E| \le 1, \\ \\ 0 & \text{otherwise}, \end{cases} \quad (2.2)$$

where $\epsilon^B(\vec{k}) = h^{BB}s(\vec{k})$, and v_m^B is the maximum velocity in the B-band. Obviously, this means setting $h^{BB} = \frac{1}{6}$ and $\epsilon^B = 0$.

Substituting (1.9) and (2.2) into (1.7) and returning to the starting point (1.1), we obtain via $\sigma_{\alpha\beta} = \sigma\delta_{\alpha\beta}$ the scalar conductivity (the notation $\sigma = \sigma[j^{(0)} + j^{(1)}]$ is also used)

$$\sigma = \hat{\sigma}\int_{-\infty}^{\infty}d\eta\left(-\frac{\partial f}{\partial\eta}\right)\{[1 + 24\sigma_1'(\eta^+) + 144(\sigma_1'(\eta^+))^2]H_0(\eta^+,\eta^-) +$$

$$+ 144[\sigma_2'(\eta^+) + 12\sigma_1'(\eta^+)\sigma_2'(\eta^+)]H_1(\eta^+,\eta^-) +$$

$$+ 4\cdot36^2(\sigma_2'(\eta^+))^2H_2(\eta^+,\eta^-) + 144\sigma_2''(\eta^+)\text{Im}\hat{F}(\eta^+) -$$

$$- \text{Re}([1 + 24\sigma_1(\eta^+) + 144(\sigma_1(\eta^+))^2]H_0(\eta^+,\eta^+) +$$

$$+ 144[\sigma_2(\eta^+) + 12\sigma_1(\eta^+)\sigma_2(\eta^+)]H_1(\eta^+,\eta^+) + \quad (2.3)$$

$$+ 4\cdot36^2(\sigma_2(\eta^+))^2H_2(\eta^+,\eta^+) + 72\sigma_2(\eta^+)\hat{F}(\eta^+))\},$$

with

$$\hat{\sigma} = \frac{2e^2 (v_m^B)^2 N}{3\pi^2 V}, \quad \sigma_\ell(z) = \sigma'_\ell(z) + i\sigma''_\ell(z), \quad (\ell=0,1,2) \quad (2.4)$$

Here the integrals

$$H_\ell(z_1,z_2) = \int_{-1}^{+1} d\xi (1-\xi^2)^{3/2} \xi^\ell \mathcal{G}(z_1;\xi)\mathcal{G}(z_2;\xi), \quad (\ell=0,1,2), \quad (2.5)$$

$$\hat{F}(z) = \int_{-1}^{+1} d\xi (1-\xi^2)^{3/2} \mathcal{G}(z;\xi) \quad (2.6)$$

are expressed in terms of the coherent Green function

$$\mathcal{G}(z;\xi) = (z - \sigma_0(z) - (1+12\sigma_1(z))\xi - 36\sigma_2(z)\xi^2)^{-1}. \quad (2.7)$$

In getting (2.3) we have used analytic properties which are satisfied by the self-energy and the coherent Green function. Indeed, the structure of the CPA equations[17] allows one to prove the relations $\sigma_\ell^*(z) = \sigma_\ell(z^*)$ and $\mathcal{G}^*(z) = \mathcal{G}(z^*)$; consequently, from (2.5) to (2.7) one gets $H_\ell^*(z_1,z_2) = H_\ell(z_1^*,z_2^*)$ and $\hat{F}^*(z) = \hat{F}(z^*)$. Note that $H_\ell(\eta^+,\eta^-)$ are real functions.

Next, we can calculate analytically the functions H_ℓ and F appearing in (2.3). Performing integration in (2.5) by the residue method, we obtain

$$H_0(\eta^+,\eta^-) = A\{1 - 2\text{Im}[-\frac{w(z_1) - w(z_2)}{z_1 - z_2}]\}, \quad (2.8)$$

$$H_1(\eta^+,\eta^-) = 2A\{\text{Re}[z_1 + z_2] - \text{Im}[-\frac{z_1 w(z_1) - z_2 w(z_2)}{z_1 - z_2}]\}, \quad (2.9)$$

$$H_2(\eta^+,\eta^-) = 2A\{\text{Re}[z_1^2 + z_2^2 + z_1 z_2 + z_1 z_2^*] + \frac{1}{2}(|z_1|^2 + |z_2|^2 - \frac{3}{2}) - \text{Im}[-\frac{z_1^2 w(z_1) - z_2^2 w(z_2)}{z_1 - z_2}]\}, \quad (2.10)$$

with

$$A = \frac{\pi}{|36\sigma_2(\eta^+)|^2}, \quad w(z) = \frac{(1-z^2)\sqrt{1-z^2}}{(z-z_1^*)(z-z_2^*)}; \quad (2.11)$$

$$H_0(\eta^+,\eta^+) = B\{1 - [p(z_1) + p(z_2) + \frac{q(z_1) - q(z_2)}{z_1 - z_2}]\}, \quad (2.12)$$

$$H_1(\eta^+,\eta^+) = B\{2(z_1+z_2) - [z_1 p(z_1) + z_2 p(z_2) - \frac{1}{2}q(z_1) - \frac{1}{2}q(z_2) + \frac{z_1 q(z_1) - z_2 q(z_2)}{z_1 - z_2}]\}, \quad (2.13)$$

$$H_2(\eta^+,\eta^+) = B\{3(z_1^2 + z_2^2) + 4z_1 z_2 - \frac{3}{2} - [z_1^2 p(z_1) + z_2^2 p(z_2) - z_1 q(z_1) - z_2 q(z_2) + \frac{z_1^2 q(z_1) - z_2^2 q(z_2)}{z_1 - z_2}]\}, \quad (2.14)$$

with

$$B = \frac{\pi}{(36\sigma_2(\eta^+))^2}, \quad p(z) = \frac{i3z\sqrt{1-z^2}}{(z_1 - z_2)^2}, \quad q(z) = \frac{i2(1-z^2)\sqrt{1-z^2}}{(z_1 - z_2)^2},$$

$$(2.15)$$

where

$$z_{1,2} = -\frac{(1+12\sigma_1)}{72\sigma_2} \pm \sqrt{\left(\frac{1+12\sigma_1}{72\sigma_2}\right) + \frac{\eta^+ - \sigma_0}{36\sigma_2}}. \quad (2.16)$$

In addition, we have to insert into (2.16) the dropped η-arguments by putting $\sigma_\ell = \sigma_\ell(\eta^+)$. Special cases as, e.g., $\sigma_2 = 0$ or $\sigma''_\ell(\eta^+) = 0$ are treated separately. The integral (2.6) can be reduced to

$$\hat{F}(\eta^+) = \frac{\pi}{2}[F_0(\eta^+) - \frac{1}{36}F_2(\eta^+)], \quad (2.17)$$

where, for the model (2.1), the quantities $F_\ell(z) = \frac{1}{N}\sum_{\vec{k}}\mathcal{G}_{\vec{k}}(z)[s(\vec{k})]^\ell$ are already known from solving the CPA problem [17].

In connection with (2.8) to (2.17), the formula (2.3) represents the analytic result for the dc conductivity directly expressed in terms of the self-energy contributions $\sigma_0, \sigma_1, \sigma_2$. For comparison, on the basis of (1.5) and (1.6) we introduce the conductivity expressions

$$\sigma[j^{(0)}] = \hat{\sigma}\int_{-\infty}^{\infty}d\eta\,(-\frac{\partial f}{\partial \eta})[H_0(\eta^+,\eta^-) - \mathrm{Re}H_0(\eta^+,\eta^+)], (2.18)$$

$$\sigma[j^{(0)} + \ll j^{(1)} \gg] = [1 + 6c(h^{AA} - h^{BB})]^2\sigma[j^{(0)}] \quad (2.19)$$

arising from the unperturbed current $j^{(0)}$ and the averaged current $j^{(0)} + \ll j^{(1)} \gg$, respectively. In view of (2.3) the quantity $\sigma[j^{(0)} + j^{(1)}] - \sigma[j^{(0)}]$ reflects the effect of the random current operator on the conductivity; additionally, the difference $\sigma[j^{(0)} + j^{(1)}] - \sigma[j^{(0)} + \ll j^{(1)} \gg]$ is a measure for the value of the statistical correlations, i.e. for the vertex corrections.

3. Numerical Results and Discussion

The numerical calculation of the conductivity is started with solving the CPA self-consistency conditions, i.e., the set of coupled integral equations [17] for $\sigma_0, \sigma_1, \sigma_2$. The input quantities are the concentration c of A atoms, the diagonal and off-diagonal randomness parameter

$$\Delta_0 = \epsilon^A, \quad \Delta_1 = 6(h^{AA} - h^{BB}), \quad (3.1)$$

respectively, and the thermal fluctuation parameter $a^\nu, \delta^\nu (\nu = A,B)$. The energy is scaled by the half-band width of the pure B-band defined in (2.1). The mean-square amplitudes [17] (with $\gamma^{(s)\nu} \equiv \gamma_n^{\nu(s)}$, $\gamma^{(s)\nu\nu} \equiv \gamma_{nm}^{\nu\nu(s)}$, see Appendix)

$$a^\nu = \langle \sum_s |\gamma^{(s)\nu}|^2 \coth(\frac{\hbar\omega_s}{2kT})\rangle_c^{|\nu}, \quad (3.2)$$

$$\delta^\nu = \frac{1}{4}\langle \sum_s |\gamma^{(s)\nu\nu}|^2 \coth(\frac{\hbar\omega_s}{2kT})\rangle_c^{|\nu}, \quad (\nu = A,B) \quad (3.3)$$

characterize thermal fluctuations of the quantities θ^ν and $\bar{\theta}^\nu$ in (1.3), respectively. Define

$$a = a^A = a^B, \quad \delta = \delta^A = \delta^B, \quad (3.4)$$

provided that the electron-phonon interaction is not affected by configurational disorder.

After having calculated the self-energies $\sigma_\ell(\eta^+)$, the η-integration in (2.3) for $T \neq 0$ is carried out numerically by a Gauss integration[18]. In any cases indicated particularly the sharply peaked function $(-\frac{\partial f}{\partial \eta})$

can be approximated by

$$-\frac{\partial f}{\partial \eta} \approx \delta(\eta - \mu) \qquad (\mu : \text{Fermi level}) \qquad (3.5)$$

according to the form for $T = 0$. This is reasonable for wide regions of the unsplit band or within the main band in the split-band case.

In investigating the conductivity versus occupied fraction of the band relationship we introduce the average number of electrons per site per spin as

$$n = \int_{-\infty}^{+\infty} f(E)\rho(E)dE, \qquad (3.6)$$

where the CPA density of states is given by (cf. (2.17))

$$\rho(E) = -\frac{1}{\pi}\text{Im}\,F_0(F + i0). \qquad (3.7)$$

To illustrate the effect of the off-diagonal randomness on the temperature dependence of the conductivity and the influence of the statistical correlations (vertex corrections) we have numerically analysed σ for some representative sets of alloy parameters. Note that the numerical results of this paper differ from those of [1-14] in two points: (i) nonvanishing vertex corrections resulting from the random current operator and (ii), unlike [12-14], off-diagonal ran-

domness of the electron-phonon interaction are taken into account. This practicable theory seems to be realistic enough to describe certain trends of experiments[19].

Sharp maxima of the conductivity at zero temperature are produced by the off-diagonal randomness as shown in Fig. 1. These "resonance" peaks arise with passing the Fermi energy through the region of maximum overlapping of the A and B-component bands. This situation is qualitatively similar to the Lifshits instability. The σ peaks disappear with increasing temperatures. Whereas σ varies by some order of magnitude, the effect of the electron-phonon scattering on the density of states is small as illustrated in Fig. 1 (c).

In Fig. (2a) the conductivity versus occupied fraction of the band curves intersect at one point (corresponding to $\mu = \Delta_0$) for all Δ_1 as already has been found earlier [8,9,11] at $T = 0$. This behaviour is here also obtained for non-zero temperatures. Analogously to ref. [11], the maxima of σ appear without divergences near to one of the band edges. Due to the statistical correlations of the random currents the vertex corrections reduce σ in the region of the conductivity maximum, i.e., $\sigma < \sigma[j^{(0)} + \ll j^{(1)} \gg]$ in Fig. 2(b),(c) Outside this region σ is enhanced by correlations, i.e., $\sigma > \sigma[j^{(0)} + \ll j^{(1)} \gg]$. On comparing σ with $\sigma[j^{(0)}]$ related to the unperturbed current $j^{(0)}$ we have $\sigma \gtrless \sigma[j^{(0)}]$ for $\Delta_1 \gtrless 0$, respectively, in analogy to $\sigma[j^{(0)} + \ll j^{(1)} \gg] \gtrless \sigma[j^{(0)}]$ according to (2.19).

By passing the Fermi energy (or occupied fraction of the band) through the conductivity minimum in Fig. 3 - not necessarily corresponding to a minimum of ρ (Fig. 3 (c))- σ
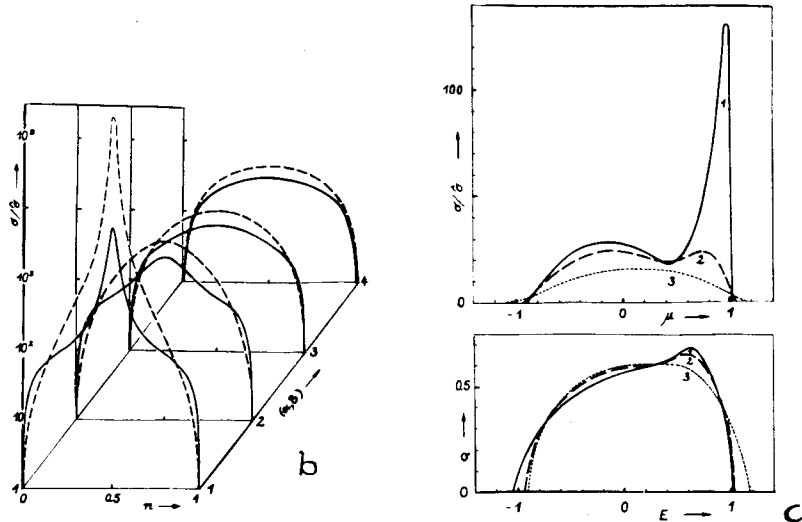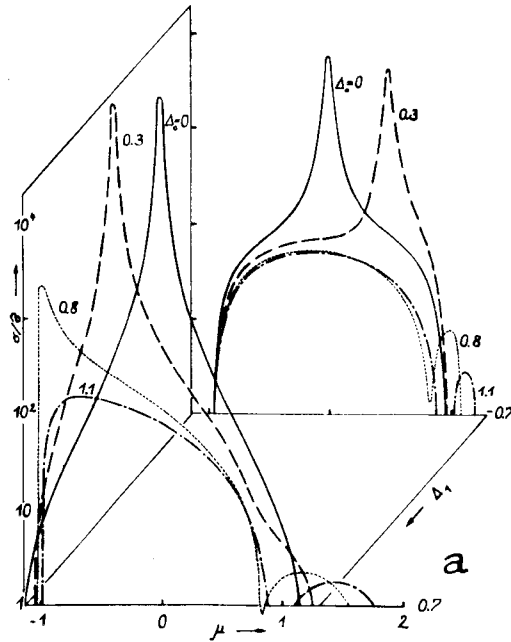
Fig. 1. dc-conductivity peak for various alloy parameters and temperatures. (a)σ vs Fermi energy μ at $T = 0K$, c =0.125. (b)σ vs occupied fraction of the band n for purely off-diagonal scattering $\Delta_0 = 0$, $\Delta_1 = 0.7$ (– – – –) and $\Delta_1 = -0.7$ (———), c = 0.125, with (1) $a = 0$, , $\delta = 0$; (2) 5×10^{-3}, 10^{-5}; (3) 1.9×10^{-2}, 5×10^{-5}; (4) 4.5×10^{-2}, 10^{-4}. (c) Density of states $\rho(E)$ and σ vs chemical potential μ at $\Delta_0 = 0.5$, $\Delta_1 = -0.5$, c = 0.25, with (1) $a = 0$, $\delta = 0$; (2) 7.5×10^{-3}, 1.5×10^{-5}; (3) 4.5×10^{-2}, 9×10^{-4}.

can increase with increasing temperatures contrary to the situation outside the minimum (compare /12, 14, 19/). In Fig. 3(b)a minimum of the σ-versus-concentration curve appears as observed in transition-metal alloys /19/. Here the possibility of anomalous temperature behaviour is also found. Deviations from a linear temperature dependence of σ are demonstrated in Fig.3(c) according to the high-temperature approximation (a, δ are proportional to T).

In the split-band case in Fig. 4, $\sigma[j^{(0)}]$ is in good agreement with the main-band conductivity σ, but not with σ on the subband. The vertex corrections reflecting the effective interaction strongly decrease the minority conductivity, expecially at non-zero temperatures. An additional structure of σ occurs in the subband in the case $a^A > a^B$, $\delta^A > \delta^B$ (cf. /17/).

This subband behaviour is investigated in detail in Fig. 5 for an alloy with $a^A = a^B$, $\delta^A = \delta^B$. The peaky structure of the density of states (Fig. 5(a)) is reproduced for the conductivity only within the approximation (3.5). By using the exact expres-
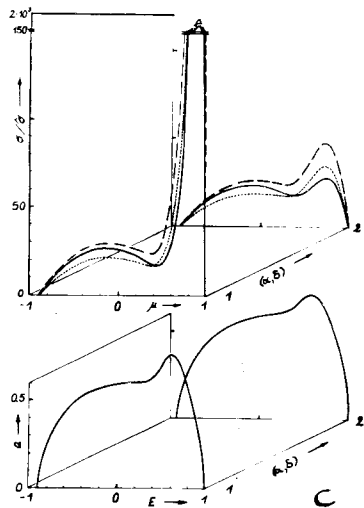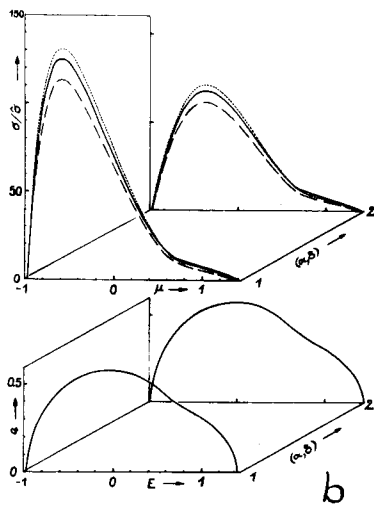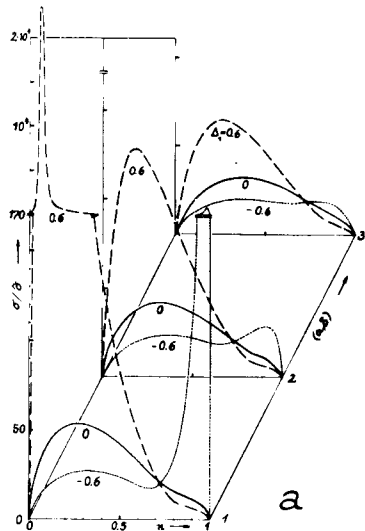
Fig. 2. Influence of thermal fluctuations and vertex corrections on the dc conductivity σ at various values of the off-diagonal randomness parameter Δ_1 with $\Delta_0 = 0.5$, $c = 0.25$, (1) $a = 0$, $\delta = 0$; (2) 7.5×10^{-3}, 1.5×10^{-5}; (3) 1.9×10^{-2}, 3.8×10^{-5}. (a) σ vs occupied fraction of the band n. (b),(c) Density of states $\rho(E)$ and σ (———), $\sigma[j^{(0)} + \ll j^{(1)} \gg]$ (····), $\sigma[j^{(0)}]$ (----) vs chemical potential μ according to (3.5) for (b) $\Delta_1 = 0.3$ and (c) $\Delta_1 = -0.6$.

sion for $(-\frac{\partial f}{\partial \eta})$ the subband fluctuations are smeared out to a very small conductivity tail. This localization effect can be expressed by a factor of about 10^2 concerning the ratio $\sigma_{\text{main b.}}^{\text{max}} / \sigma_{\text{subb.}}^{\text{max}}$ at $T \neq 0$ (factor of 25 at $T = 0$ in Fig. 5 (b)). The extreme decrease of the minority conductivity is caused by the combined effect of the electron-phonon scattering and statistical correlations.

Appendix

Electron-Phonon Interaction in Off-Diagonal Random Model Systems

The model system considered is composed of two types of atoms, A and B, which are randomly placed on N sites of a regular lattice. A single level according to a tightly bound electron state is associated with each of the atoms. The one-electron Hamiltonian in the field of a fixed configuration $\{\nu\}$ of ions

$$H_e + H_{int} = -\frac{\hbar^2}{2m} \Delta_{\vec{r}} + \sum_n V^\nu (\vec{r} - \tilde{\vec{R}}_n), (\nu = A, B) \quad (A.1)$$
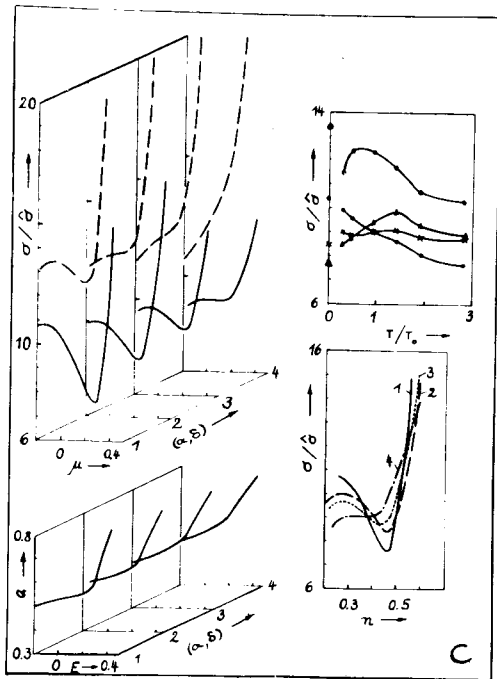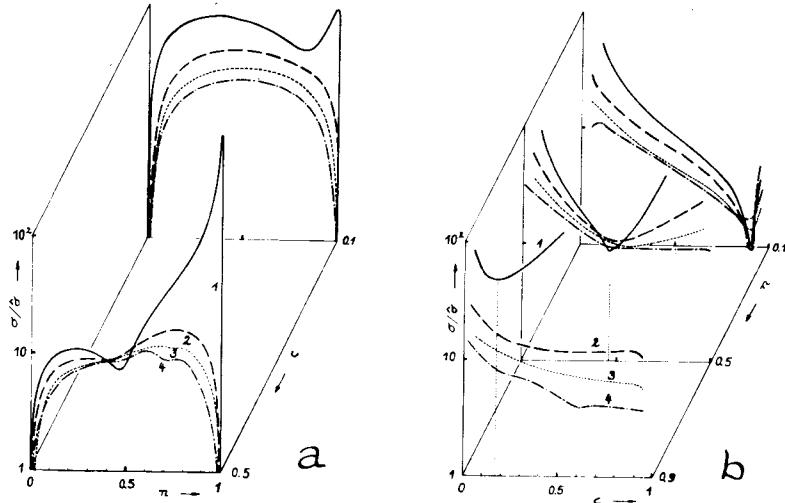
a

b

c

Fig. 3. dc conductivity σ at various alloy concentrations and temperatures for $\Delta_0 = 0.5$, $\Delta_1 = -0.5$. (a) σ vs occupied fraction of the band n and (b) σ vs concentration c with (1) $a = 0$, $\delta = 0$; (2) 1.9×10^{-2}, 3.8×10^{-5}; (3) 3.8×10^{-2}, 7.5×10^{-5}; (4) 5.6×10^{-2}, 1.1×10^{-4}. (c) Density of states $\rho(E)$, σ (———) and $\sigma[j^{(0)}]$ (– – –) vs chemical potential μ, and σ vs n with (1) $a = 0$, $\delta = 0$; (2) 5.6×10^{-3}, 1.1×10^{-5}; (3) 9.4×10^{-3}, 1.9×10^{-5}; (4) 1.9×10^{-2}, 3.8×10^{-5}; σ vs temperature T for n $= 0.55$ (-O-O-O), 0.45 (Δ-Δ-Δ), 0.4 (x-x-x), and 0.3 (●-●-●) near the dc conductivity minimum. Here (3.5) and $a = a_0 T/T_0$ with $a_0 = 0.02$ are used.
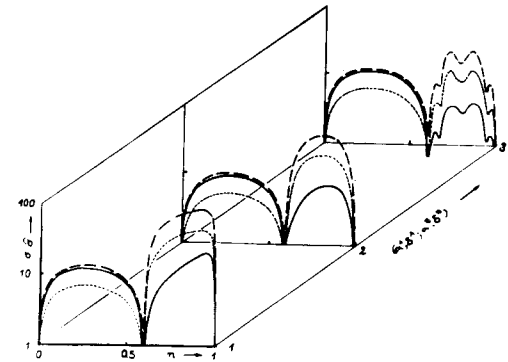
Fig. 4. dc conductivity σ for configuration-dependent fluctuation parameters. σ (———), $\sigma[j^{(0)} + \ll j^{(1)} \gg]$ (·····) and $\sigma[j^{(0)}]$ (– – –) vc occupied fraction of the band n according to (3.5) for $\Delta_0 = 0.9$, $\Delta_1 = -0.7$, c $= 0.4$ with (1) $a^A = 0$, $\delta^A = 0$, $a^B = 0$, $\delta^B = 0$; (2) 7.5×10^{-3}, 1.5×10^{-5}, 2.2×10^{-2}, 4.5×10^{-5}; (3) 2.2×10^{-2}, 4.5×10^{-5}, 7.5×10^{-3}, 1.5×10^{-5}.

a

b
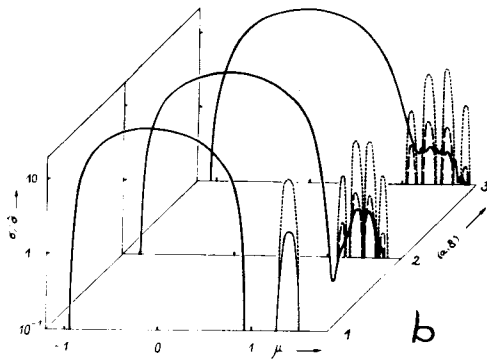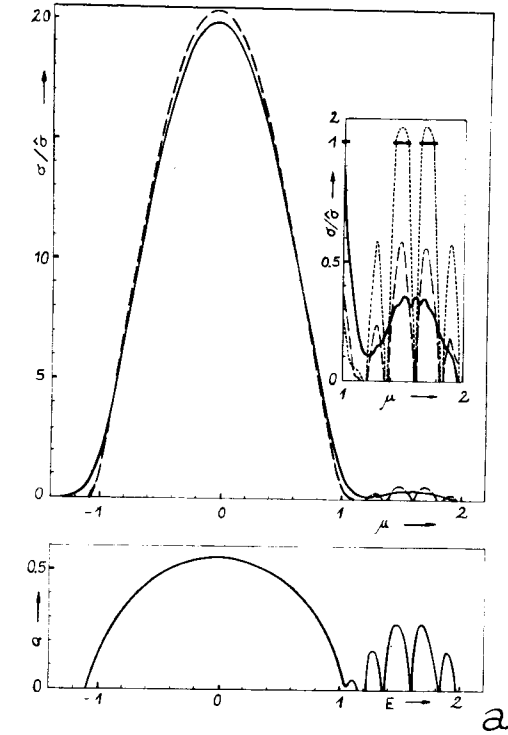
Fig. 5. Effect of the vertex corrections on the temperature-dependent dc conductivity σ in the split-band case. σ (———), σ (– – –) according to (3.5), and $\sigma[j^{(0)}+\ll j^{(1)}\gg]$ (....) to (3.5) are plotted for $c=0.125$. (a) Density of states $\rho(E)$ and σ vs chemical potential μ at $\Delta_0 =1.5$, $\Delta_1 =-0.5$, $a =4.5\times10^{-2}$, $\delta = 9\times10^{-5}$. (b) σ vs μ at $\Delta_0 =1.3$, $\Delta_1 =-0.7$ with (1) $a =0$, $\delta =0$; (2) 2.2×10^{-2}, 4.5×10^{-5}; (3) 4.5×10^{-2}, 9×10^{-5}.

includes the electron-lattice interaction in terms of $V^\nu(\vec{r}-\vec{R}_n)$ describing the interaction of the electron with a given ν ion at position $\vec{R}_n = \vec{R}_n + \vec{x}_n$. Here $\vec{x}_n$ is the displacement vector from the equilibrium ion position $\vec{R}_n$ at n-th site. By assuming first-order displacements we get

$$V^\nu(\vec{r}-\tilde{\vec{R}}_n) = V^\nu(\vec{r}-\vec{R}_n) - \nabla V^\nu(\vec{r}-\vec{R}_n)\cdot\vec{x}_n. \qquad (A.2)$$

The harmonic motion of the atoms in the configuration $\{\nu\}$ is described by the Hamiltonian

$$H_{\ell at} = \sum_{\substack{n\\ \alpha}} \frac{p_{n\alpha}^2}{2M_n^\nu} + \frac{1}{2}\sum_{\substack{nm\\ \alpha\beta}} \Phi_{\substack{nm\\ \alpha\beta}}^{\nu\mu} x_{n\alpha} x_{m\beta}, \quad (\nu,\mu = A,B), \qquad (A.3)$$

where $p_{n\alpha}$ is the α-component of the momentum of the n-th atom, M_n^ν is the mass of the n-th atom, and $\Phi_{\substack{nm\\ \alpha\beta}}^{\nu\mu}$ are the harmonic force constants. The superscripts ν,μ refer to the type of atom at lattice sites n and m, respectively. The total Hamiltonian within $\{\nu\}$ is then $H = H_e + H_{int} + H_{\ell at}$.

Introducing phonon creation (b_s^+) and annihilation (b_s) operators we can write (cf. /20/)

$$x_n^{}_\alpha = \sum_s \sqrt{\frac{\hbar}{2\omega_s M_n^\nu}} [W_n^{(s)}{}_\alpha b_s + (W_n^{(s)}{}_\alpha)^* b_s^+], \qquad (A.4)$$

$$p_n^{}_\alpha = -i\sum_s \sqrt{\frac{\hbar\omega_s M_n^\nu}{2}} [W_n^{(s)}{}_\alpha b_s - (W_n^{(s)}{}_\alpha)^* b_s^+], \qquad (A.5)$$

where the quantum number s runs over 3N normal modes of the vibrational subsystem. Here ω_s and $W_n^{(s)}{}_\alpha$ are the eigenvalues and eigenvectors of the random dynamical matrix, respectively; this means setting

$$\sum_{\substack{m \\ \beta}} [\omega_s^2 \delta_{nm}\delta_{\alpha\beta} - (M_n^\nu M_m^\nu)^{-1/2}\Phi_{nm}^{\nu\mu}{}_{\alpha\beta}] W_m^{(s)}{}_\beta = 0. \qquad (A.6)$$

Note that the special case of the ordered system is also included by replacing ω_s and $W_n^{(s)}{}_\alpha$ by $\omega_{\vec{q}\lambda}$ and $W_{n\vec{q}}{}_\alpha = \frac{1}{\sqrt{N}} e_{\vec{q}\lambda}{}_\alpha e^{i\vec{q}\vec{R}_n}$, respectively. Then $\vec{q}$ is the phonon wavevector, λ is the vibrational branch index, $e_{\vec{q}\lambda}{}_\alpha$ denotes the α-component of the polarization vector.

Within a slightly modified tight-binding approximation one allows the electrons to follow adiabatically the vibrating ions. To define the tight-binding basis we introduce the Wannier function $\phi^\nu(\vec{r} - \tilde{\vec{R}}_n)$ (abbreviated by $|\tilde{n}\rangle$) satisfying the Schrödinger equation

$$[-\frac{\hbar^2}{2m}\Delta_{\vec{r}} + V^\nu(\vec{r}-\tilde{\vec{R}}_n)]\phi(\vec{r}-\tilde{\vec{R}}_n) = \tilde{\epsilon}^\nu(\vec{x}_n)\phi^\nu(\vec{r}-\tilde{\vec{R}}_n), \qquad (A.7)$$

provided that the tightly bound wave function follows the displaced ν ion without appreciable deformation. For small displacements the orthogonality relation of the Wannier functions remains valid. The quantities in (A.7) with respect to the equilibrium lattice are denoted by ϵ_n^ν and $\phi^\nu(\vec{r} - \vec{R}_n)$ (abbreviated by $|n\rangle$).

Expanding the integral

$$\langle\tilde{n}|H_e + H_{int}|\tilde{m}\rangle = \qquad (A.8)$$
$$= \int \phi^{\nu*}(\vec{r}-\tilde{\vec{R}}_n)[-\frac{\hbar^2}{2m}\Delta_{\vec{r}} + \sum_{n'} V^{\nu'}(\vec{r}-\tilde{\vec{R}}_{n'})]\phi^\mu(\vec{r}-\tilde{\vec{R}}_m)d\vec{r}$$

to first order in the ion-displacement coordinates, one gets with (A.2) and (A.7) by neglecting pure and degenerate three-center integrals the expression

$$\langle\tilde{n}|H_e + H_{int}|\tilde{m}\rangle = [\epsilon_n^\nu - \vec{d}_{nn}^{\nu\nu} \cdot \vec{x}_n]\delta_{nm} +$$
$$+ [h_{nm}^{\nu\mu} + \vec{g}_{nm}^{\nu\mu}\cdot(\vec{x}_n - \vec{x}_m) - \qquad (A.9)$$
$$- \frac{1}{2}(\vec{d}_{nm}^{\nu\mu} \cdot \vec{x}_n + (\vec{d}_{mn}^{\mu\nu})^*\cdot \vec{x}_m)](1-\delta_{nm}),$$

where

$$\vec{d}_{nm}^{\nu\mu} = \langle n|\nabla V_n^\nu|m\rangle =$$
$$\qquad (A.10)$$
$$= \int \phi^{\nu*}(\vec{r} - \vec{R}_n)\nabla V^\nu(\vec{r}-\vec{R}_n)\phi^\mu(\vec{r} - \vec{R}_m)d\vec{r},$$

$$\epsilon_n^\nu = \langle n|V_n^\nu|n\rangle, \quad h_{nm}^{\nu\mu} = \frac{1}{2}[\langle n|V_n^\nu|m\rangle + (\langle m|V_m^\mu|n\rangle)^*], \qquad (A.11)$$

$$\vec{g}_{nm}^{\nu\mu} = [\frac{\partial}{\partial r} h_{nm}^{\nu\mu} (r)]_{r=a} (\frac{\vec{R}_n - \vec{R}_m}{a}). \qquad (A.12)$$

The last relation was obtained on taking the overlap integral $h_{nm}^{\nu\mu}$ as a function of $|\vec{R}_n - \vec{R}_m|$; a is the lattice spacing. The two-center integrals in (A.9) are restricted to the nearest neighbours (n.n.). Note that $\tilde{\epsilon}^{\nu}(\vec{x}_n)$ in (A.7) can be expressed in terms of (A.10) and (A.11) as

$$\tilde{\epsilon}^{\nu}(\vec{x}_n) = \epsilon_n^{\nu} - \vec{d}_{nn}^{\nu\nu} \cdot \vec{x}_n .$$

Combining (A.3) and (A.9) with (A.4) and (A.5), the total Hamiltonian for a particular set $\{\nu\}$ reads

$$H = \sum_n \epsilon_n^{\nu} a_n^+ a_n + \sum_{\substack{nm \\ (m \neq n: n.n.)}} h_{nm}^{\nu\mu} a_n^+ a_m +$$
$$+ \sum_n a_n^+ a_n \sum_s [\gamma_n^{\nu(s)} b_s + (\gamma_n^{\nu(s)})^* b_s^+] + \qquad (A.13)$$
$$+ \sum_{\substack{nm \\ (m \neq n: n.n.)}} a_n^+ a_m \sum_s [\gamma_{nm}^{\nu\mu(s)} b_s + (\gamma_{mn}^{\mu\nu(s)})^* b_s^+] + \sum_s \hbar\omega_s (b_s^+ b_s + \frac{1}{2}),$$

where

$$\gamma_n^{\nu(s)} = - \sqrt{\frac{\hbar}{2\omega_s M_n^{\nu}}} \vec{d}_{nn}^{\nu\nu} \cdot \vec{W}_n^{(s)} , \qquad (A.14)$$

$$\gamma_{nm}^{\nu\mu(s)} = -\sqrt{\frac{\hbar}{2\omega_s}}[(\frac{1}{2}\vec{d}_{nm}^{\nu\mu} - \vec{g}_{nm}^{\nu\mu}) \cdot \frac{\vec{W}_n^{(s)}}{\sqrt{M_n^{\nu}}} + (\frac{1}{2}\vec{d}_{mn}^{\mu\nu} - \vec{g}_{mn}^{\mu\nu})^* \cdot \frac{\vec{W}_m^{(s)}}{\sqrt{M_m^{\mu}}}] . \qquad (A.15)$$

Here a_n^+ and a_n are operators creating and annihilating an electron in the Wannier state at site n according to the modified

tight-binding approximation. Especially, the contribution with $\vec{g}_{nm}^{\nu\mu}$ in (A.15) reflecting phonon-modulated hopping was derived from the Wannier functions centered at the instantaneous position of the ion. In this way, the atomic aspect of the electron is emphasized by (A.13) in order to describe, e.g., random transition-metal alloys. The local (or shortly-ranged) randomness of $\epsilon_n^{\nu}, h_{nm}^{\nu\mu}, \gamma_n^{\nu(s)}$ and $\gamma_{nm}^{\nu\mu(s)}$

is pointed out by setting $\nu,\mu = A,B$. Moreover, the electron-phonon coupling elements $\gamma_n^{\nu(s)}$ and $\gamma_{nm}^{\nu\mu(s)}$ depend implicitly on the total configuration $\{\nu\}$ via the phonon quantities ω_s and $W_{\frac{n}{a}}^{(s)}$.

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