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Spin Fluctuations in Alloys with Random Transfer

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The local spin fluctuation theory proposed by Hasegawa is extended to binary alloys with random transfer of the additive type. Spin fluctuations and alloy disorder are treated within an extended coherent potential approximation (ODCPA). The dc conductivity σ, including CPA vertex corrections, is derived via density–density susceptibility from the functional integral scheme. In the paramagnetic region model calculations are presented for the averaged local moment, σ, density of states, and the distribution function of spin fluctuations.

Die lokale Spinfluktuationstheorie von Hasegawa wird für binäre Legierungen mit stochastischem Transfer vom additiven Typ erweitert. Spinfluktuationen und Legierungsunordnung werden in einer erweiterten Näherung des kohärenten Potentials (ODCPA) behandelt. Die dc-Leitfähigkeit σ wird unter Berücksichtigung von CPA-Vertexkorrekturen über die Dichte–Dichte-Suszeptibilität aus dem funktionalen Schema abgeleitet. Modellrechnungen werden im paramagnetischen Bereich für das gemittelte lokale Moment, sowie σ, Zustandsdichte und Verteilungsfunktion der Spinschwankungen vorgestellt.

1. Introduction

There is much current interest in the investigation of electric and magnetic properties of transition metals and transition metal alloys [1 to 11]. Their theoretical description within a band theory (for these substances the Fermi level lies in narrow d-bands) is based on the Hubbard model [12]. As is well known the Hartree-Fock (HF) approximation of the model gives good results in the ground state but fails at finite temperatures. To explain for instance the low Curie temperatures T_C in spite of the large exchange splitting energies and the Curie Weiss behaviour of the susceptibility in ferromagnetic metals, as well as the existence of local moments above T_C, it is indispensable to take into account low-energy excitations of the spin density. Moriya [9] has pointed out that the nature of these fluctuations can vary in a region between the local moment and the weakly ferromagnetic case. A powerful method to include the fluctuations theoretically is the functional integral technique developed by Evenson et al. [13]. It forms the foundation for the spin fluctuation theory proposed by Hubbard [1] and Hasegawa [3], using an approach from the local limit in real space. Their theory was also applied to antiferromagnetic [3] and paramagnetic [10] transition metals. The first steps in treating alloys were taken by Hasegawa [5] (diagonal disorder) and Kakehashi [8] (inclusion of multiplicative random hopping).

In this paper we extend the spin fluctuation theory to alloys with additive off-diagonal randomness (ODR), which allows us to investigate the interlock of correlations and randomness. We proceed as follows. After a brief review of the functional integral method (Section 2), the determination of the $\boldsymbol{k}$-dependent self-energy of an averaged system takes place within the ODCPA, using Hasegawa's decoupling scheme in the CPA equations [5] (Section 3). Consistently with the treatment of the electron

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correlation in Section 3 we calculate the dc conductivity at finite temperatures from the density–density susceptibility in Section 4. CPA vertex corrections due to ODR are included. Numerical results are presented and discussed in Section 5.

2. Functional Integral Approach

To describe the magnetic properties of a substitutionally disordered alloy, we start with the one-band Hubbard Hamiltonian

$$H^{\{\nu\}} = \sum_{i\sigma} \varepsilon_i^\nu c_{i\sigma}^+ c_{i\sigma} + \sum_{\substack{ij\sigma \\ (i\neq j)}} t_{ij}^{\nu\mu} c_{i\sigma}^+ c_{j\sigma} + \sum_i U_i^\nu n_{i\uparrow} n_{i\downarrow} \tag{1}$$

for an arbitrary configuration $\{\nu\}$; ν and μ refer to the two kinds of atoms (A or B), which are (according to their concentrations x^ν) randomly distributed on the sites i and j of a simple cubic lattice. ε_i^ν and U_i^ν denote the atomic energy and the intra-atomic Coulomb repulsion, respectively. The random hopping energies $t_{ij}^{\nu\mu}$ are restricted to nearest neighbours (n.n.). The operator $c_{i\sigma}^+$ ($c_{i\sigma}$) creates (destroys) a spin σ electron in the Wannier state at site i and $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$. Using the decomposition $n_{i\uparrow} n_{i\downarrow} = \frac{1}{4}[(n_{i\uparrow} + n_{i\downarrow})^2 - (n_{i\uparrow} - n_{i\downarrow})^2]$ [14] and performing the Hubbard-Stratonovich transformation [15] the generating functional Z for fermion Green functions can be expressed in the charge neutrality limit by a path integral over anticommuting (Grassmann) variables and space- and time-dependent fields as

$$Z^{\{\nu\}}[\bar\eta\eta] = \int D\bar c\, Dc\, D\xi\, e^{A_L^{\{\nu\}}[\bar c c,\xi] + \bar c\eta + \bar\eta c}, \tag{2}$$

with

$$A_L^{\{\nu\}} = \int_0^\beta d\tau \sum_{ij\sigma} \bar c_{i\sigma}(\tau)\,[-\partial_\tau \delta_{ij} - [H_L^{\{\nu\}}(\tau)]_{ij\sigma}]\, c_{j\sigma}(\tau) - \int_0^\beta \sum_i \left\{ \frac{U_i^\nu}{4} \xi_i^2(\tau) - n_i^\nu w_i^\nu(\xi_i(\tau)) \right\}, \tag{3}$$

$$[H_L^{\{\nu\}}(\tau)]_{ij\sigma} = \left(\varepsilon_i^\nu + w_i^\nu(\xi_i(\tau)) - \sigma \frac{U_i^\nu}{2} \xi_i(\tau) \right) \delta_{ij} + t_{ij}(1 - \delta_{ij}) \tag{4}$$

and the abbreviation $\bar c\eta + \bar\eta c = \int_0^\beta d\tau \sum_{i\sigma} (\bar c_{i\sigma}(\tau)\, \eta_{i\sigma}(\tau) + \bar\eta_{i\sigma}(\tau)\, c_{i\sigma}(\tau))$. Here $c_{i\sigma}(\tau)$ ($\bar c_{i\sigma}(\tau)$) corresponds to the operator $c_{i\sigma}(c_{i\sigma}^+)$, τ denotes the imaginary time, $\beta = 1/(k_B T)$, k_B is the Boltzmann constant and T the absolute temperature. The random action (3) involves the linearized Hamiltonian H_L, whose matrix elements (4) are explicitly spin dependent. H_L describes noninteracting electrons which are influenced in their motion by a kind of exchange field configuration [1]. The charge potentials $w_i^\nu(\xi)$ have been chosen to conserve the mean electron number n_i^ν at ν-sites independent of the ξ-field fluctuation. Through $Z^{\{\nu\}}[0,0] = Z^{\{\nu\}} = \mathrm{Tr}\, e^{-\beta H^{\{\nu\}}}$ the generating functional (2) is related to the partition function Z in the limit of vanishing external sources η [16]. In view of (4) it is convenient to introduce the Green function through

$$\sum_{m\sigma'} (-\partial_\tau \delta_{im} - [H_L^{\{\nu\}}(\tau)]_{\substack{im \\ \sigma}})\, \delta_{\sigma\sigma'} [G_\xi^{\{\nu\}}(\tau,\tau')]_{\substack{mj \\ \sigma'\sigma''}} = \delta_{ij}\delta_{\sigma\sigma'}\delta(\tau - \tau'). \tag{5}$$

In an alternative way G can be derived from (2) by functional derivation with respect to η and $\bar\eta$. Performing the integration in (2) over the fermion fields, one obtains

$$Z^{\{\nu\}}[\bar\eta\eta] = \int D\xi\, e^{\mathrm{Tr}\ln[-G_\xi^{\{\nu\}-1}] - \left[\frac{U^\nu}{4}\xi^2 - n^\nu w^\nu(\xi)\right] - \bar\eta G_\xi^{\{\nu\}}\eta}. \tag{6}$$

Treating the fields $\xi_i(\tau)$ in the static approximation, we get from (6) for the partition function

$$Z^{\{\nu\}} = \int \mathrm{D}\xi \, \mathrm{e}^{-\beta\psi^{\{\nu\}}[\xi]} , \tag{7}$$

with

$$\psi^{\{\nu\}} = \sum_i \left[\frac{U_i^\nu}{4}\,\xi_i^2 - n_i^\nu u_i^\nu(\xi_i)\right] + \int_{-\infty}^{\infty} f(E)\,\frac{\mathrm{Im}}{\pi}\,\mathrm{Tr}\ln\left(-G_\xi^{\{\nu\}}(E^+)^{-1}\right)\mathrm{d}E , \tag{8}$$

where Tr means the trace in spin and lattice space (N sites), $f(E)$ is the Fermi distribution function, μ the chemical potential, and $E^+ = E + i0$. Note that (7) involves the full N-centre problem. With regard to (7) the average of some electronic quantity K can be expressed as

$$\overline{\langle K^{\{\nu\}}\rangle_{\mathrm{td}}^{\mathrm{c}}} = \overline{\langle K^{\{\nu\}}[\xi]\rangle^{\mathrm{c}}} = \overline{\left[\frac{\int \mathrm{D}\xi K^{\{\nu\}}[\xi]\,\mathrm{e}^{-\beta\psi[\xi]}}{Z^{\{\nu\}}}\right]^{\mathrm{c}}} , \tag{9}$$

taking into account the equivalence of functionals and operators. Here $\langle\ldots\rangle_{\mathrm{td}}$, $\langle\ldots\rangle$, and $\overline{(\ldots)^{\mathrm{c}}}$ denote the thermodynamic, functional, and configurational averages, respectively.

3. ODCPA Treatment of Spin Fluctuations

The ODR in (1) is chosen to be of the form $t^{\mathrm{AB}} = \frac{1}{2}(t^{\mathrm{AA}} + t^{\mathrm{BB}})$, which implies $t_{ij}^{\nu\mu} = t^{\mathrm{BB}} + t_i^\nu + t_j^\mu$ (cf. [17]). The random parameters are subject to the probability distribution

$$P(\varepsilon_i^\nu, t_i^\nu, U_i^\nu) = x^{\mathrm{A}}\,\delta(\varepsilon_i^\nu - \varepsilon^{\mathrm{A}}, t_i^\nu + \tfrac{1}{2}(t^{\mathrm{BB}} - t^{\mathrm{AA}}), U_i^\nu - U^{\mathrm{A}}) + x^{\mathrm{B}}\,\delta(\varepsilon_i^\nu, t_i^\nu, U_i^\nu - U^{\mathrm{B}}) , \tag{10}$$

where we have separated from $H^{\{\nu\}}$ a periodic part associated with the pure B-crystal. This means $\overline{(\ldots)^{\mathrm{c}}} = \int \mathrm{d}\varepsilon_i^\nu\,\mathrm{d}t_i^\nu\,\mathrm{d}U_i^\nu\,P(\varepsilon_i^\nu, t_i^\nu, U_i^\nu)\ldots$ According to (10) the matrix elements of $G_\xi^{\{\nu\}-1}$, which we need to calculate ψ, take the form

$$[G_\xi^{\{\nu\}}(E^+)]_{\substack{nm\\ \sigma}}^{-1} = \mathcal{G}_{\substack{nm\\ \sigma}}^{-1}(E^+) - \sum_i \{[V_i^\nu]_{\substack{nm\\ \sigma}} - [\Sigma_i(E^+)]_{\substack{nm\\ \sigma}}\} \tag{11}$$

with

$$[V_i^\nu]_{\substack{nm\\ \sigma}} = \left(\varepsilon_i^\nu - \varepsilon^{\mathrm{B}} + u_i^\nu(\xi_i) - \sigma\,\frac{U_i^\nu}{2}\,\xi_i\right)\delta_{in}\delta_{nm} + t_i^\nu(\delta_{im} + \delta_{in})\,(1 - \delta_{nm}) , \tag{12}$$

$$\mathcal{G}_{\substack{nm\\ \sigma}}(z) = \frac{1}{N}\sum_{\boldsymbol{k}} \mathrm{e}^{-i\boldsymbol{k}(\boldsymbol{R}_n - \boldsymbol{R}_m)}\,\mathcal{G}_{\boldsymbol{k}\sigma}(z) , \tag{13}$$

$$\mathcal{G}_{\boldsymbol{k}\sigma}(z) = [z - \varepsilon^{\mathrm{B}} - t^{\mathrm{BB}}\,s(\boldsymbol{k}) - \Sigma_\sigma(\boldsymbol{k}, z)]^{-1} , \tag{14}$$

and $s(\boldsymbol{k}) = \sum_{(j\neq i;\,\mathrm{n.n.})} \mathrm{e}^{-i\boldsymbol{k}(\boldsymbol{R}_j - \boldsymbol{R}_i)}$. Here we have introduced the propagator $\mathcal{G}$ and the $\boldsymbol{k}$-dependent self-energy $\Sigma_\sigma(\boldsymbol{k}, z)$ corresponding to an averaged system. To keep the evaluation of (9) tractable we make the following approximations: (i) Σ and $\mathcal{G}$ are determined within a single-site approximation, the ODCPA. (ii) In accordance with (i) we carry out the decomposition $\psi^{\{\nu\}}[\xi] \to \sum_i \psi_i^\nu(\xi_i)$, that means (9) becomes a product of N identical integrals. (iii) We use Hasegawa's [5] decoupling approximations $\langle\xi^{2n}\rangle^\nu \approx (\langle\xi^2\rangle^\nu)^n$ and $\langle\xi^{2n+1}\rangle^\nu \approx (\langle\xi^2\rangle^\nu)^n\,\langle\xi\rangle^\nu$, which transform the system into an effective Ising model [8]. Thus, in view of (i) to (iii), (9) becomes

$$\overline{\langle K^\nu(\xi)\rangle^{\mathrm{c}}} = \sum_{\substack{\nu\\ s=\pm 1}} x^\nu w_s^\nu K^\nu(sq^\nu) , \tag{15}$$

with

$$w_s^\nu = \frac{1}{2}\left(1 + s\frac{\langle\xi\rangle^\nu}{q^\nu}\right) \tag{16}$$

and $q^\nu = \sqrt{\langle\xi^2\rangle^\nu}$ (cf. [8]). $\langle\ldots\rangle^\nu$ denotes the conditional average $\int \mathrm{d}\xi_i\, C_i^\nu(\xi_i)\ldots$ at ν-sites, with respect to the local distribution function

$$C_i^\nu(\xi_i) = \mathrm{e}^{-\beta\psi_i^\nu(\xi_i)}\,[\int \mathrm{d}\xi_i\, \mathrm{e}^{-\beta\psi_i(\xi_i)}]^{-1} \tag{17}$$

for the auxiliary fields. Using the Dyson equation for G, (8) becomes

$$\psi_i^\nu(\xi_i) = \frac{U_i^\nu}{4}\xi_i^2 - n_i^\nu u_i^\nu(\xi_i) + \int_{-\infty}^{\infty} \mathrm{d}E\, f(E)\,\frac{\mathrm{Im}}{\pi}\,\mathrm{tr}\ln\left(1 - \mathcal{G}(V - \Sigma)\right), \tag{18}$$

where an irrelevant factor is dropped. This is the alloy-analogy picture: an impurity site i is embedded in an otherwise effective CPA medium. Note that in contrast to only diagonal disorder [5] we have to compute the trace tr in the Bloch representation, because the perturbation $(V - \Sigma)$ is nonlocal in Wannier space. Its matrix elements are given by

$$[V_{i\sigma}^\nu(\xi) - \Sigma_{i\sigma}]_{\boldsymbol{k}\boldsymbol{k}'} = \frac{1}{N}\,\mathrm{e}^{-i\boldsymbol{R}_i(\boldsymbol{k}-\boldsymbol{k}')}\,\{\Delta_{0\sigma}^\nu(\xi) + \Delta_{1\sigma}^\nu(s(\boldsymbol{k}) + s(\boldsymbol{k}')) + \Delta_{2\sigma}s(\boldsymbol{k})\,s(\boldsymbol{k}')\} \tag{19}$$

with the abbreviations

$$\begin{aligned}
\Delta_{0\sigma}^\nu(\xi) &= \varepsilon_i^\nu - \varepsilon^{\mathrm{B}} + u_i^\nu(\xi_i) - \sigma\frac{U_i^\nu}{2}\xi_i - \Sigma_{0\sigma}\,,\\
\Delta_{1\sigma}^\nu &= t_i^\nu - \Sigma_{1\sigma}\,,\\
\Delta_{2\sigma} &= -\Sigma_{2\sigma}\,,
\end{aligned} \tag{20}$$

corresponding to the full self-energy $\Sigma_\sigma(\boldsymbol{k}, z) = \Sigma_{0\sigma} + 2\Sigma_{1\sigma}s(\boldsymbol{k}) + \Sigma_{2\sigma}s(\boldsymbol{k})^2$. Expanding the logarithm and performing the trace in (18) we get

$$\psi_i^\nu(\xi_i) = \frac{U_i^\nu}{4}\xi_i^2 - n_i^\nu u_i^\nu(\xi_i) - \int_{-\infty}^{\infty}\mathrm{d}E\, f(E)\,\frac{\mathrm{Im}}{\pi}\sum_\sigma\sum_{p=1}^{\infty}\frac{1}{p}\times$$

$$\times\,(\Omega_{0\sigma}^{(p)\nu}(E^+)\,F_{0\sigma}(E^+) + 2\Omega_{1\sigma}^{(p)\nu}(E^+)\,F_{1\sigma}(E^+) + \Omega_{2\sigma}^{(p)\nu}(E^+)\,F_{2\sigma}(E^+))\,, \tag{21}$$

where

$$F_{l\sigma} = \frac{1}{N}\sum_{\boldsymbol{k}}\mathcal{G}_{\boldsymbol{k}\sigma}[s(\boldsymbol{k})]^l \qquad (l = 0, 1, 2)\,. \tag{22}$$

The recursion formulas for the $\Omega_{l\sigma}^{(p)\nu}$ are given in the Appendix. They show the coupling of the fluctuations in a cluster consisting of site i and all its n.n. The self-energy parts $\Sigma_{l\sigma}$ result from six coupled t-matrix equations

$$\sum_{\nu s} x^\nu w_s^\nu \tau_{l\sigma}^\nu(sq^\nu) = 0\,, \tag{23}$$

where the explicit expressions of $\tau_{l\sigma}$ are also listed in the Appendix. Taking into account (i) to (iii) the self-consistency equations (23) can be obtained from functional differentiation of the free energy with respect to the averaged propagator $\mathcal{G}$. In the case of only diagonal disorder (23) reduces to (2.6) in [5]. With the local Green function

$$G_{ii\sigma}^\nu(\xi) = F_{0\sigma} + F_{0\sigma}^2\tau_{0\sigma}^\nu(\xi) + 2F_{1\sigma}\tau_{1\sigma}^\nu(\xi) + F_{1\sigma}^2\tau_{2\sigma}^\nu(\xi) \tag{24}$$

one gets, for the partial electron numbers at ν-sites,

$$n_{i\sigma}^{\nu}(\xi) = \int_{-\infty}^{\infty} \mathrm{d}E\, f(E)\, \frac{(-)}{\pi}\, \mathrm{Im}\, G_{ii\sigma}^{\nu}(\xi, E^{+}) \,. \tag{25}$$

Thus, in view of (24) and (25), the charge neutrality condition takes the form

$$n_i^{\nu} = \sum_{\sigma} n_{i\sigma}^{\nu}(\xi) \tag{26}$$

and the chemical potential is fixed by the requirement

$$n = \int_{\infty-}^{\infty} \mathrm{d}E\, f(E)\, \frac{(-)}{\pi} \sum_{\sigma} \mathrm{Im}\, F_{0\sigma}(E^{+}) \,. \tag{27}$$

To compute averages using (15), it is therefore necessary first to solve (23), (26), (27) together with (17) self-consistently for a given T. Then, employing (25), the averaged magnetization m and the root-mean-square local moment m_{loc} are given by

$$m = \sum_{\nu} x^{\nu} \sum_{s} w_s^{\nu} \sum_{\sigma} \sigma n_{i\sigma}^{\nu}(sq^{\nu}) \;, \tag{28}$$

$$m_{\mathrm{loc}} = \sum_{\nu} x^{\nu} \left[\sum_{s} w_s^{\nu} \left[\sum_{\sigma} \sigma n_{i\sigma}^{\nu}(sq^{\nu}) \right]^2 \right]^{1/2} . \tag{29}$$

Using general relations of the functional technique [13], which are also hold in the approximations (i) to (iii), we can calculate m and m_{loc} in an alternative way,

$$m = \overline{\langle \xi \rangle^{\nu}}^{\mathrm{c}} \;, \tag{30}$$

$$m_{\mathrm{loc}} = \overline{\left[\langle \xi^2 \rangle^{\nu} - \frac{2}{\beta U^{\nu}} \right]^{1/2}}^{\mathrm{c}} \,. \tag{31}$$

Thus it is possible to evaluate the self-consistent loop (23), (26) to (31) for the determination of $\Sigma_{l\sigma}$.

4. Calculation of the Temperature-Dependent DC Conductivity

Our starting point is the density–density susceptibility

$$\chi_{ij}(\tau, \tau') = -\sum_{\sigma} \overline{\langle T_\tau n_{i\sigma}(\tau')\, n_{j\sigma}(\tau) \rangle^{\mathrm{c}}}^{\mathrm{td}} = -\sum_{\sigma} \overline{\langle \underset{\xi}{G_{ji\sigma}^{\{\nu\}}}(\tau', \tau)\, \underset{\xi}{G_{j,\sigma}^{\{\nu\}}}(\tau, \tau') \rangle^{\mathrm{c}}} \tag{32}$$

of noninteracting electrons within a ξ-field configuration. The second equality in (32) follows from functional differentiation of (6) with respect to the fermion sources. T_τ is Wick's time ordering operator and the functional average is performed after setting the external sources equal to zero. By using the relation between $\sigma(0)$ and the current density–current density response function [18], as well as the continuity equation, one gets for the static electric conductivity

$$\sigma(0) = -\,\mathrm{Re} \lim_{\omega \to 0} \lim_{\boldsymbol{q} \to \boldsymbol{0}} \frac{i e^2 \omega}{q^2}\, \chi(\boldsymbol{q}, \omega) \,, \tag{33}$$

where the Fourier transform of (32) reads

$$\chi(\boldsymbol{q}, \omega_m) = -\overline{\left\langle \frac{1}{N\beta} \sum_{\omega_n} \sum_{ij\sigma} \underset{\xi}{G_{ij\sigma}^{\{\nu\}}}(\omega_n)\, \underset{\xi}{G_{ji}^{\{\nu\}}}(\omega_n + \omega_m)\, \mathrm{e}^{-i\boldsymbol{q}(\boldsymbol{R}_i - \boldsymbol{R}_j)} \right\rangle^{\mathrm{c}}} \tag{34}$$

($\omega_m = 2m\pi T$ and $\omega_n = (2n+1)\,\pi T$ are the Matsubara frequencies). The averaged two-particle correlation function related to (32) obeys the integral equation

$$\mathcal{G}^{\mathrm{II}}_{imjn}(z_1, z_2) = \overline{\langle G^{\{\nu\}}_{ij}(z_1)\, G^{\{\nu\}}_{mn}(z_2)\rangle}^{\mathrm{c}} = \overline{\langle G^{\{\nu\}}_{ij}(z_1)\rangle}^{\mathrm{c}}\,\overline{\langle G^{\{\nu\}}_{mn}(z_2)\rangle}^{\mathrm{c}} + \\ + \sum_{lprs} \overline{\langle G^{\{\nu\}}_{il}(z_1)\rangle}^{\mathrm{c}}\,\overline{\langle G^{\{\nu\}}_{sn}(z_2)\rangle}^{\mathrm{c}}\, \frac{\delta\Sigma_{ls}(z_1)}{\delta\overline{\langle G^{\{\nu\}}_{pr}(z_2)\rangle}^{\mathrm{c}}}\, \mathcal{G}^{\mathrm{II}}_{pmjr}(z_1, z_2)\,. \tag{35}$$

To proceed we expand $\chi(\boldsymbol{q}, \omega_m)$ after analytical continuation, in view of (33), to lowest nonvanishing order in q and ω, extracting a pole structure. This allows us to solve (35), even in the presence of ODR, if we make the approximations (i) to (iii) for the functional average (i.e. $\langle\ldots\rangle \to \langle\ldots\rangle^{\nu}$). For (34) we obtain (cf. [19])

$$\chi(\boldsymbol{q}, \omega) = \frac{1}{2\pi i} \sum_{\sigma} \int_{-\infty}^{\infty} \left\{ f(E) \left(-\frac{\partial F_{0\sigma}(E^+)}{\partial E} \right) - f(E+\omega) \left(-\frac{\partial F_{0\sigma}(E^-)}{\mathrm{d}E} \right) - \right. \\ \left. - 2i\big(f(E+\omega) - f(E)\big) \frac{\operatorname{Im} F_{0\sigma}(E^+)}{\omega + iD_\sigma(E)\, q^2} \right\} \mathrm{d}E \tag{36}$$

with the prescription

$$D_\sigma(E) = -\frac{1}{2 \operatorname{Im} F_{0\sigma}(E^+)} \lim_{\omega\to 0} \lim_{\boldsymbol{q}\to \boldsymbol{0}} \left[\frac{\omega^2}{Nq^2} \sum_{\boldsymbol{k}} \big(\mathcal{G}^{\mathrm{II}}_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k},\sigma}(\boldsymbol{q}, E^+ + \omega, E^-) - \right. \\ \left. - \mathcal{G}^{\mathrm{II}}_{\boldsymbol{k},\boldsymbol{k},\sigma}(0, E^+ + \omega, E^-) \big) \right] \tag{37}$$

for the calculation of the diffusion coefficient. The explicit expression of D,

$$D_\sigma(E) = \frac{1}{12 \operatorname{Im} F_{0\sigma}(E^+)} \left[\Pi_\sigma(E^+, E^+) + \Pi_\sigma(E^-, E^-) - 2\Pi_\sigma(E^+, E^-) \right] \tag{38}$$

with

$$\Pi_\sigma(z_1, z_2) = \frac{1}{N} \sum_{\boldsymbol{k}} \left\{ \mathcal{G}_{\boldsymbol{k}\sigma}(z_1) \mathcal{G}_{\boldsymbol{k}\sigma}(z_2) \left[\nabla_{\boldsymbol{k}} \left(t^{\mathrm{BB}} s(\boldsymbol{k}) + \frac{1}{2} \big(\Sigma_\sigma(\boldsymbol{k}, z_1) + \Sigma_\sigma(\boldsymbol{k}, z_2) \big) \right) \right]^2 + \right. \\ \left. + \left[\sigma_{2\sigma}(z_1)\, \mathcal{G}_{\boldsymbol{k}}(z_2) + \sigma_{2\sigma}(z_2)\, \mathcal{G}_{\boldsymbol{k}\sigma}(z_1) \right] \left[\nabla_{\boldsymbol{k}} s(\boldsymbol{k}) \right]^2 \right\} \tag{39}$$

was given in [18], however, in (39) the $\mathcal{G}$'s are renormalized due to spin fluctuations. So for the conductivity we get the final result

$$\sigma(0) = \frac{e^2}{k_{\mathrm{B}} T} \sum_{\sigma} \int_{-\infty}^{\infty} f(E)\,(1 - f(E))\, \varrho_\sigma(E)\, D_\sigma(E)\, \mathrm{d}E\,, \tag{40}$$

where $\varrho_\sigma(E) = -1/\pi \operatorname{Im} F_{0\sigma}(E^+)$ denotes the density of states. In the case of vanishing Coulomb interaction (40) corresponds to the solution of the conductivity problem obtained in [20, 21]. It is easy to see that for σ the limit $T \to 0$ gives the HF result.

5. Numerical Results and Discussion

The next step is to present model calculations, illustrating the influence of ODR on the quantities calculated in Sections 3 and 4. In this paper we restrict ourselves mainly to the paramagnetic regime, calculations in the ferromagnetic phase are in prepara-

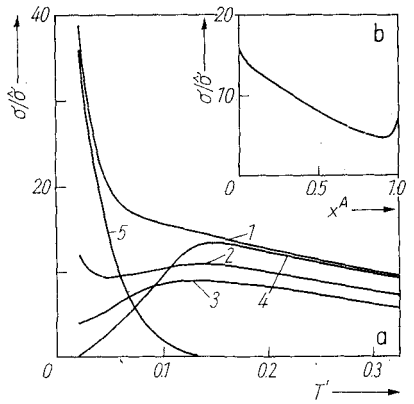

Fig. 1. dc conductivity σ (in units of $\hat{\sigma}$) at various reduced temperatures $T'=k_B T/2W^B$ and concentrations x^A for the parameter set $P = (\varepsilon^A, \varepsilon^B, W^A, W^B, U^A, U^B) = (-0.5, -0.5, 0.5, 1, 1, 1)$ and $n = 1$. a) σ vs. T' for (1) $x^A = 0$, (2) 0.3, (3) 0.5, (4) 1 whereas curve 5 denotes the case $x^A = 0$ using the approximation $f(E) \approx \theta(-E)$; b) σ vs. x^A at $T' = 0.0861$

tion. For simplicity we use the semielliptic model density

$$\varrho^B(E) = \frac{1}{N}\sum_{\boldsymbol{k}} \delta(E - s(\boldsymbol{k})\, t^{BB}) = \frac{2}{\pi W^B}\left[1 - \left(\frac{E}{W^B}\right)^2\right]^{1/2} \theta(W^B - |E|) \tag{41}$$

for the unperturbed B-band, which implies

$$\frac{1}{N}\sum_{\boldsymbol{k}} \delta(E - t^{BB}s(\boldsymbol{k}))\,(t^{BB}\nabla_{\boldsymbol{k}} s(\boldsymbol{k}))^2 = \frac{2v_m^B}{\pi W^B}\left[1 - \left(\frac{E}{W^B}\right)^2\right]^{3/2} \theta(W^B - |E|)\,. \tag{42}$$

Thus, the $\boldsymbol{k}$-summations in (22) and, what is important, in (39) can be performed analytically. Here $W^B = 6t^{BB}$ is the half-bandwidth, $\varepsilon^B = 0$, and v_m^B denotes the maximum velocity in the B-band.

Fig. 1 a shows the temperature dependence of σ, scaled by $\hat{\sigma} = e^2(v_m^B)^2/(3\pi)$, for the half-filled band at various alloy concentrations. Depending on U^ν/W^ν (i.e. band splitting or not), σ tends to zero (infinity) in the limit $x^A \to 1(0)$ if $T \to 0$. This is due to the fact that for $T \to 0$ the theory gives the HF result, that means for the pure system there exists no scattering mechanism, implying a real Σ. At high temperatures the difference between the cases $x^A = 0$ and $x^A = 1$ vanishes and σ decreases with increasing temperature. This decay can be also observed in the region $0 < x^\nu < 1$. But, owing to the additional scattering mechanism and the vertex corrections by statistical correlations, σ is strongly reduced, a fact which is illustrated in Fig. 1 b at fixed temperature. It should be noted that in contrast to [3] the system undergoes no sharp metal–insulator transition if the Fermi distribution is correctly taken into account (compare curves 1 and 5).

For better insight, in Fig. 2 $\varrho(E)$, the integrand of (40) and the distribution functions $C^\nu(\xi)$ are given referring to curve 2 in Fig. 1. At low temperatures $C^\nu(\xi)$ behaves differently at A- and B-sites (owing to U^ν/W^ν). While $C^B(\xi)$ exhibits only one broad maximum $C^A(\xi)$ has a double-maximum structure. With increasing temperature the two peaks merge into a single peak, a behaviour in agreement with the results obtained by Sakoh and Shimizu [22] for the pure system. But in contrast to their observation $\varrho(E)$ splits off at higher temperatures (Fig. 2 a). This is due to Hasegawa's decoupling scheme in the CPA equations, leading to an Ising-like system, where in accordance with (31) the length q^ν of the Ising spins increases with T (cf. Fig. 3). The contribution of several electronic states to σ is pictured in Fig. 2 b.

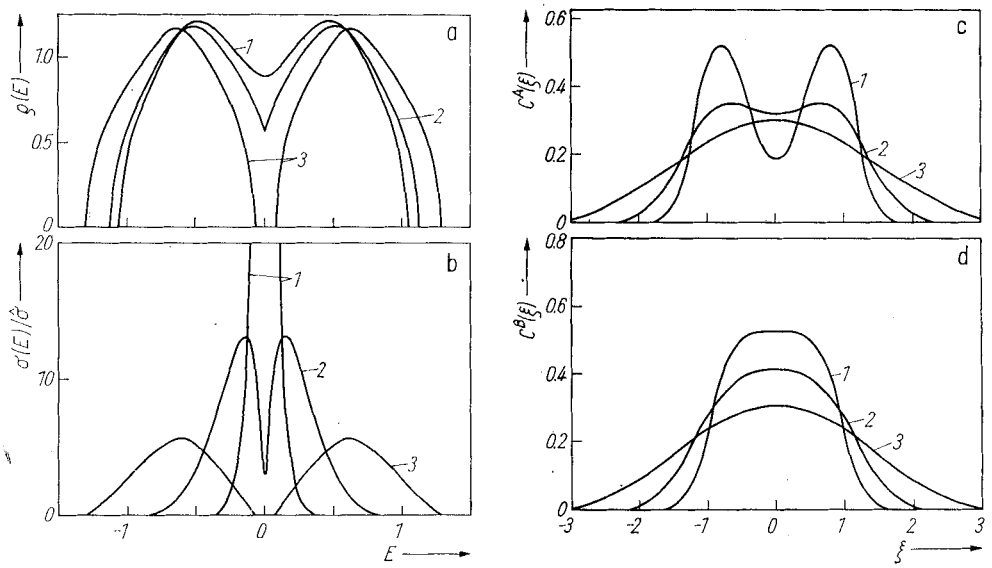

Fig. 2. Temperature variations of a) the density of states $\varrho(E)$, b) the integrand of the conductivity formula (40), $\sigma(E)$; the reduced distribution function $C^{\nu}(\xi)$ at c) A-sites and d) B-sites for the set P used in Fig. 1 with $n = 1$ and $x^{\mathrm{A}} = 0.3$ at (1) $T'' = 0.0215$, (2) 0.0645, (3) 0.301

In Fig. 3 the temperature variation of the local moment is shown. For $n = 1$ the ground state is antiferromagnetically ordered and the results are only of physical significance above the Néel temperature. First we should emphasize that, different from the situation for σ, the influence of ODR is important only at low temperatures. Taking into account the Fermi distribution which was neglected in [3, 10] we obtain

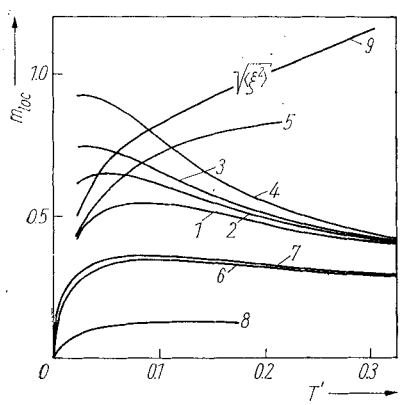

Fig. 3

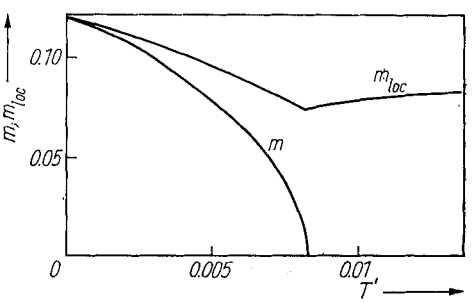

Fig.4

Fig. 3. Temperature dependence of the local moment m_{loc} for the set P and $n = 1$: (1) $x^{\mathrm{A}} = 0$, (2) 0.3, (3) 0.5, (4) 1; $n = 0.5$: (6) $x^{\mathrm{A}} = 0.3$, (7) 0.5; $n = 0.2$: (8) $x^{\mathrm{A}} = 0.3$. Employing $f(E) \approx \approx \theta(-E)$ curve 5 is plotted in comparison to curve 1. Curve 9 shows $\sqrt{\langle \xi^2 \rangle}$ vs. T'' at $n = 1$ and $x^{\mathrm{A}} = 0$

Fig. 4. Averaged magnetization m and local moment m_{loc} vs. reduced temperature T' for a pure B-system using the unperturbed density of states (41). Parameters are $n = 0.12$ and $U^{\mathrm{B}}/W^{\mathrm{B}} = 4$

a decay of m_{loc} in the high-temperature region. For comparison curve 5 has been calculated in the approximation $f(E) \approx \theta(\mu - E)$. If the ground state is paramagnetic we have $m_{\mathrm{loc}}(T = 0) = 0$ in the static approximation and an increase with rising temperature (i.e. the local moments are thermally induced). Similar results were found for paramagnetic transition metals by Evangelou et al. [10].

In order to clarify the influence of the model density, in Fig. 4 the T-dependences of m and m_{loc} are shown using the bell-shaped band (41), where the electron number and $m(T = 0)$ correspond to Ni. We get the expected reduction of the Curie temperature, ($T_{\mathrm{C}} = 460$ K if $W^{\mathrm{B}} = 2.38$ eV) and the slight increases of m_{loc} above T_{C}. However, $m(T)$ shows an apparent deviation from the Brillouin curve contrary to the case where a more realistic sharply peaked density of states is used (cf. [4]).

A more elaborated evaluation of the ferromagnetic phase including ODR would be an interesting subject of further investigations.

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Appendix

The quantities $\Omega_{l\sigma}^{(p)\nu}(\xi)$ from (21) are given through the following recursion formulas:

$$\Omega_{0\sigma}^{(p+1)\nu}(\xi) = (\Delta_{0\sigma}^{\nu}(\xi)\, F_{0\sigma} + \Delta_{1\sigma}^{\nu} F_{1\sigma})\, \Omega_{0\sigma}^{(p)\nu}(\xi) + (\Delta_{0\sigma}^{\nu}(\xi)\, F_{1\sigma} + \Delta_{1\sigma}^{\nu} F_{2\sigma})\, \Omega_{1\sigma}^{(p)\nu}(\xi)\,, \tag{A1}$$

$$\begin{aligned}\Omega_{1\sigma}^{(p+1)\nu}(\xi) &= (\Delta_{0\sigma}^{\nu}(\xi)\, F_{0\sigma} + \Delta_{1\sigma}^{\nu} F_{1\sigma})\, \Omega_{1\sigma}^{(p)\nu}(\xi) + (\Delta_{0\sigma}^{\nu}(\xi)\, F_{1\sigma} + \Delta_{1\sigma}^{\nu} F_{2\sigma})\, \Omega_{2\sigma}^{(p)\nu}(\xi) \\ &= (\Delta_{1\sigma}^{\nu} F_{0\sigma} + \Delta_{2\sigma} F_{1\sigma})\, \Omega_{0\sigma}^{(p)\nu}(\xi) + (\Delta_{1\sigma}^{\nu} F_{1\sigma} + \Delta_{2\sigma} F_{2\sigma})\, \Omega_{1\sigma}^{(p)\nu}(\xi)\,, \end{aligned} \tag{A2}$$

$$\Omega_{2\sigma}^{(p+1)\nu}(\xi) = (\Delta_{1\sigma}^{\nu} F_{0\sigma} + \Delta_{2\sigma} F_{1\sigma})\, \Omega_{1\sigma}^{(p)\nu}(\xi) + (\Delta_{1\sigma}^{\nu} F_{1\sigma} + \Delta_{2\sigma} F_{2\sigma})\, \Omega_{2\sigma}^{(p)\nu}(\xi)\,, \tag{A3}$$

$$\Omega_{0\sigma}^{(1)\nu}(\xi) = \Delta_{0\sigma}^{\nu}(\xi)\,, \qquad \Omega_{1\sigma}^{(1)\nu} = \Delta_{1\sigma}\,, \qquad \Omega_{2\sigma}^{(1)\nu} = \Delta_{2\sigma}\,.$$

The local t-matrices in (23) are given by (cf. [17])

$$\tau_{l\sigma}^{\nu}(sq^{\nu}) = t_{l\sigma}^{\nu}(sq^{\nu})\,[1 - d_{\sigma}^{\nu}(sq^{\nu})]^{-1}\,, \tag{A4}$$

with

$$t_0^{\nu}(sq^{\nu}) = \Delta_{0\sigma}^{\nu}(sq^{\nu}) - (\Delta_{1\sigma}^{\nu})^2 F_{2\sigma} - \Delta_{0\sigma}^{\nu}(sq^{\nu})\, \Delta_{2\sigma} F_{2\sigma}\,, \tag{A5}$$

$$t_1^{\nu}(sq^{\nu}) = \Delta_{1\sigma}^{\nu} - (\Delta_{1\sigma}^{\nu})^2 F_{1\sigma} + \Delta_{0\sigma}^{\nu}(sq^{\nu})\, \Delta_{2\sigma} F_{1\sigma}\,, \tag{A6}$$

$$t_2^{\nu}(sq^{\nu}) = \Delta_{2\sigma} + (\Delta_{1\sigma}^{\nu})^2 F_{0\sigma} - \Delta_{0\sigma}^{\nu}(sq^{\nu})\, \Delta_{2\sigma} F_{0\sigma}\,, \tag{A7}$$

$$\begin{aligned} d_{\sigma}^{\nu}(sq^{\nu}) = {} & \Delta_{0\sigma}^{\nu}(sq^{\nu})\, F_{0\sigma} + 2\Delta_{1\sigma}^{\nu} F_{0\sigma} + \Delta_{2\sigma} F_{2\sigma} - \\ & - [(\Delta_{1\sigma}^{\nu})^2 - \Delta_{0\sigma}^{\nu}(sq^{\nu})\, \Delta_{2\sigma}]\,[F_{1\sigma}^2 - F_{0\sigma} F_{2\sigma}]. \end{aligned} \tag{A8}$$

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