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T-MATRIX CALCULATION OF ITINERANT-ELECTRON FERROMAGNETISM IN OFF-DIAGONAL DISORDERED ALLOYS

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The transverse spin current susceptibility of disordered Hubbard ferromagnets is examined employing a Bethe–Salpeter-like equation. A magnon scattering contribution to the spin wave stiffness coefficient is deduced by averaging out off-diagonal disorder in the additive limit. Self-consistent numerical solutions of the coherent ladder approximation are presented in the ferromagnetic case for densities of states, self-energies, and local two--particle T-matrices. The application to NiPt alloys brings out the effects of electron correlations and random hopping integrals.

1. *Introduction*

The ferromagnetic state in transition metal alloys is strongly affected by off-diagonal disorder provided that, e.g., $3d$- and $5d$- substituents participate in the itinerancy. Attempts to calculate the spin wave stiffness constant D (i.e., the magnon energy $\omega_q = Dq^2$ for small q) for such systems require the simultaneous treatment of off-diagonal randomness and electron-electron interaction within a tight-binding model. Working along this line a random phase decoupling scheme was proposed in [1], which makes an additive ansatz for the hopping integrals and circumvents the coherent potential approximation (CPA). Using the Hartree-Fock approximation (HFA) for the Hubbard-type interaction an additional magnon scattering contribution to D was derived in [2] for a general type of off--diagonal disorder. In the approach [3] D was renormalized by vertex corrections due to the random transverse spin current and by electron-electron correlations within the coherent ladder approximation (CLA) [4], where the off-diagonal disorder is restricted to the additive limit.

In the present paper the average exchange stiffness D in [3] is completed in the sense of [2] by a magnon scattering contribution, the explicit form of which evolves from the additivity of the current operator. Numerical CLA results reflecting the dynamical aspect of the ferromagnetism are applied to NiPt alloys. Here the emphasis is on the overall self--consistency of the spectral properties arising from both one- and two-particle (T-matrix) scatterings.

2. *Configurational average of the transverse spin current susceptibility*

The itinerant d-electron ferromagnetism in A_cB_{1-c} alloys can be found on the Hubbard model Hamiltonian including both diagonal and off-diagonal disorder as

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

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is the creation (annihilation) operator for a spin σ electron in the Wannier state at lattice site i, and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. For the alloy configuration $\{\nu\}$ the hopping integrals $t_{ij}^{\nu\mu}$, the atomic energy ε_i^{ν}, and the intraatomic Coulomb interaction U_i^{ν} are labeled by $\nu\,(\mu)$ referring to the atomic species (ν, $\mu = A, B$) located at site $i\,(j)$. To examine the dynamics of the ferromagnetic state we first consider at zero temperature the transverse spin current-spin current response function [3]

$$q^2 \chi_J^{+-}(\vec{q}, \omega) = -\frac{i}{N} \int \frac{dE}{2\pi} \langle \mathrm{tr}\, \{ \Lambda_{\uparrow\downarrow}^{\{\nu\}}(E, E+\omega; \vec{q}) G_{\downarrow}^{\{\nu\}}(E+\omega) \lambda^{\{\nu\}}(-\vec{q}) G_{\uparrow}^{\{\nu\}}(E) \} \rangle_c. \tag{2}$$

Here N is the number of lattice sites, the trace means summation (without spin) over the one-particle states, $G_{\sigma}^{\{\nu\}}$ is the one-particle causal Green function within $\{\nu\}$, and $\langle \ldots \rangle_c$ denotes the configuration average. The effective spin-flip vertex $\Lambda_{\substack{ij \\ \uparrow\downarrow}}^{\{\nu\}}$ satisfies the integral equation

$$\Lambda_{\substack{ij \\ \uparrow\downarrow}}^{\{\nu\}}(E, E+\omega; \vec{q}) = \lambda_{ij}^{\nu\mu}(\vec{q}) - \delta_{ij} \int \frac{d\bar{E}}{2\pi}\, i I_{\substack{i \\ \uparrow\downarrow\downarrow\uparrow}}^{\{\nu\}}(E, \bar{E}+\omega; \omega) \sum_{mn} G_{im\uparrow}^{\{\nu\}}(\bar{E})$$
$$\times \Lambda_{\substack{mn \\ \uparrow\downarrow}}^{\{\nu\}}(\bar{E}, \bar{E}+\omega; \vec{q}) G_{ni\downarrow}^{\{\nu\}}(\bar{E}+\omega), \tag{3}$$

where

$$\lambda_{ij}^{\nu\mu}(\vec{q}) = t_{ij}^{\nu\mu}(e^{-i\vec{q}\vec{R}_i} - e^{-i\vec{q}\vec{R}_j}), \tag{4}$$

and $\vec{R}_i$ is the position vector. The irreducible particle-hole vertex $I_i^{\{\nu\}}$ is assumed to be site-diagonal. Taking (2) to order q^2, i.e. putting $\lambda^{\{\nu\}}(\vec{q}) = \vec{q} \cdot \vec{j}^{\{\nu\}}$ and $\Lambda_{\uparrow\downarrow}^{\{\nu\}}(E, E+\omega; \vec{q}) = \vec{q} \cdot \vec{\Lambda}_{\uparrow\downarrow}(E, E+\omega)$, we get with (3) and (4) by using cubic symmetry the following expressions

$$\chi_J^{+-}(\vec{q} = 0, \omega) = \frac{i}{3N} \int \frac{dE}{2\pi} \langle \mathrm{tr}\, \{ \vec{j}^{\{\nu\}} G_{\downarrow}^{\{\nu\}}(E+\omega) \vec{j}^{\{\nu\}} G_{\uparrow}^{\{\nu\}}(E) \} \rangle_c + \tilde{\chi}_J^{+-}(\vec{q} = 0, \omega), \tag{5}$$

$$\tilde{\chi}_J^{+-}(\vec{q} = 0, \omega) = \frac{i}{3N} \int \frac{dE}{2\pi} \left\langle \sum_{imn} \vec{\Lambda}_{\substack{ii \\ \uparrow\downarrow}}^{\{\nu\}}(E, E+\omega) G_{im\downarrow}^{\{\nu\}}(E+\omega) \vec{j}_{mn}^{\,\mu\nu} G_{ni\uparrow}^{\{\nu\}}(E) \right\rangle_c, \tag{6}$$

$$\vec{\Lambda}^{\{\nu\}}_{\substack{ij\\ \uparrow\downarrow}}(E, E+\omega) = \vec{j}^{\,\nu\mu}_{ij} - \delta_{ij} \int \frac{d\bar{E}}{2\pi}\, i I^{\{\nu\}}_{\substack{i\\ \uparrow\downarrow\downarrow\uparrow}}(E, \bar{E}+\omega; \omega) \sum_{mn} G^{\{\nu\}}_{im\uparrow}(\bar{E}) \vec{\Lambda}^{\{\nu\}}_{\substack{mn\\ \uparrow\downarrow}}(\bar{E}, \bar{E}+\omega) G^{\{\nu\}}_{ni\downarrow}(\bar{E}+\omega), \tag{7}$$

$$\vec{j}^{\,\nu\mu}_{ij} = -i t^{\nu\mu}_{ij}(\vec{R}_i - \vec{R}_j). \tag{8}$$

In an earlier study [3] the contribution (6) was neglected by a factorization ansatz. To give a lowest-order estimation of the vertex corrections hidden in $\tilde{\chi}_J^{+-}$ we expand the random quantities around their configuration averages. Moreover, we make the replacement $I^{\{\nu\}}_{\substack{i\\ \uparrow\downarrow\downarrow\uparrow}} = -\langle U^{\nu}_i \rangle_c = -\bar{U}$ (or one may choose an appropriate T-matrix value $-\langle T^{\nu}_i \rangle_c$). Then by performing a double Fourier transform we solve (7), yielding $\vec{\Lambda}^{\{\nu\}}_{\vec{q}\uparrow\downarrow} = \sum_i \vec{\Lambda}^{\{\nu\}}_{\substack{ii\\ \uparrow\downarrow}} e^{-iqR_i}$ in first order of $\vec{j}^{\{\nu\}}$ as

$$\vec{\Lambda}^{\{\nu\}}_{\vec{q}\uparrow\downarrow} = \frac{\bar{U}i}{N} \sum \int \frac{d\bar{E}}{2\pi} \mathcal{G}_{\vec{k}+\vec{q}\uparrow}(\bar{E}) \vec{\Lambda}^{\{\nu\}}_{\substack{\vec{k}+\vec{q}\vec{k}\\ \uparrow\downarrow}} \mathcal{G}_{\vec{k}\downarrow}(\bar{E}) = \frac{\dfrac{\bar{U}i}{N} \sum\limits_{\vec{k}} \displaystyle\int \frac{dE}{2\pi} \mathcal{G}_{\vec{k}+\vec{q}\uparrow}(E) \vec{j}^{\{\nu\}}_{\vec{k}+\vec{q}\vec{k}} \mathcal{G}_{\vec{k}\downarrow}(E+\omega)}{1 - \dfrac{\bar{U}i}{N} \sum\limits_{\vec{k}} \displaystyle\int \frac{dE}{2\pi} \mathcal{G}_{\vec{k}+\vec{q}\uparrow}(E) \mathcal{G}_{\vec{k}\downarrow}(E)}, \tag{9}$$

where $\mathcal{G}_\sigma(z) = \langle G^{\{\nu\}}_\sigma(z) \rangle_c$ is the averaged Green function. In order to get the simplest non-trivial approximation of $\tilde{\chi}_J^{+-}$ we have to replace the $G^{\{\nu\}}_\sigma$ in (6) by $\mathcal{G}_\sigma$, so that we are left with fluctuating terms in the second order. Thus, in momentum representation, (6) reads

$$\tilde{\chi}_J^{+-}(\vec{q} = 0, \omega) = \frac{i}{3N} \int \frac{dE}{2\pi} \frac{1}{N^2} \left\langle \sum_{\vec{k}\vec{q}} \vec{\Lambda}^{\{\nu\}}_{-\vec{q}\uparrow\downarrow} \mathcal{G}_{\vec{k}+\vec{q}\downarrow}(E+\omega) \vec{j}^{\{\nu\}}_{\vec{k}+\vec{q}\vec{k}} \mathcal{G}_{\vec{k}\uparrow}(E) \right\rangle_c. \tag{10}$$

By inserting (9) into (10) we arrive at

$$\lim_{\omega \to 0} \tilde{\chi}_J^{+-}(\vec{q} = 0, \omega) = \frac{\bar{U}}{3N^2} \sum_{\vec{q}} \frac{\left\langle \left| \dfrac{i}{N} \sum\limits_{\vec{k}} \displaystyle\int \frac{dE}{2\pi} \mathcal{G}_{\vec{k}\uparrow}(E) \vec{j}^{\{\nu\}}_{\vec{k}\vec{k}+\vec{q}} \mathcal{G}_{\vec{k}+\vec{q}\downarrow}(E) \right|^2 \right\rangle_c}{1 - \dfrac{\bar{U}i}{N} \sum\limits_{\vec{k}} \displaystyle\int \frac{dE}{2\pi} \mathcal{G}_{\vec{k}+\vec{q}\downarrow}(E) \mathcal{G}_{\vec{k}\uparrow}(E)}. \tag{11}$$

Within the HFA treatment [2] an expression analogous to (11) was derived in the weak--scattering approximation, and the correspondence with virtual magnon scattering processes was discussed. According to the spatial inhomogeneity of $\vec{j}^{\,\nu\mu}_{ij}$, the vertex correction in (11) appears as a consequence of the off-diagonal randomness. For pure or only diagonal random systems the result (11) tends to zero due to time-reversal symmetry.

Let us carry out the configurational averaging in (11) for an alloy with off-diagona disorder in the additive limit

$$t_{ij}^{\nu\mu} = t^{BB}+t_i^{\nu}+t_i^{\mu} \ (i, j\colon \text{n.n}); \qquad t_i^{\nu} = \begin{cases} \frac{1}{2}(t^{AA}-t^{BB}), & \nu = A \\ 0, & \nu = B \end{cases} \tag{12}$$

where only nearest-neighbour (n.n.) transfer integrals $t_{ij}^{\nu\mu}$ (shortly $t^{\nu\mu}$) are included. This allows us to write $\vec{j}^{\{\nu\}} = \vec{j}^{(0)}+\vec{j}^{(1)\{\nu\}}$ with $\vec{j}^{(1)\{\nu\}} = \sum_i \vec{j}_i^{(1)\{\nu\}}$, where only the random part $\vec{j}^{(1)\{\nu\}}$ gives a nonzero contribution to (11). The current $\vec{j}_i^{(1)\nu}$ obtained from (8) and (12) takes the Fourier transform

$$\vec{j}_{ikk'}^{(1)\nu} \equiv \langle \vec{k}|j_i^{(1)\nu}|\vec{k}'\rangle = e^{-i(\vec{k}-\vec{k}')\vec{R}_i} t_i^{\nu}(\nabla_{\vec{k}} s(\vec{k})+\nabla_{\vec{k}'} s(\vec{k}')), \tag{13}$$

where

$$s(\vec{k}) = \sum_{j(\neq i)}' e^{i\vec{k}(\vec{R}_i-\vec{R}_j)}. \tag{14}$$

In view of (11) we must average products of the type $\sum_{mn} \langle\langle \vec{k}|\vec{j}_m^{(1)\mu}|\vec{k}+\vec{q}\rangle \langle \vec{k}'+\vec{q}|\vec{j}_n^{(1)\nu}|\vec{k}'\rangle\rangle_c$. According to the off-diagonal CPA [5] the decoupling scheme

$$\langle \vec{j}_m^{(1)\mu}\vec{j}_n^{(1)\nu}\rangle_c = \begin{cases} \langle(\vec{j}_m^{(1)\mu})^2\rangle_c, & m = n \\ \langle \vec{j}_m^{(1)\mu}\rangle_c \langle \vec{j}_n^{(1)\nu}\rangle_c, & m \neq n \end{cases} \tag{15}$$

leads with (13) and (14) to

$$\sum_m \langle\langle \vec{k}|\vec{j}_m^{(1)\mu}|\vec{k}+\vec{q}\rangle \langle \vec{k}'+\vec{q}|\vec{j}_m^{(1)\mu}|\vec{k}'\rangle\rangle_c = N\langle t_m^{\mu 2}\rangle_c(\nabla_{\vec{k}} s(\vec{k})+\nabla_{\vec{k}+\vec{q}} s(\vec{k}+\vec{q}))$$

$$\times(\nabla_{\vec{k}'+\vec{q}} s(\vec{k}'+\vec{q})+\nabla_{\vec{k}'} s(\vec{k}')). \tag{16}$$

The terms $m \neq n$ in (15) give rise to $\sum_m \langle\langle \vec{k}|\vec{j}_m^{(1)\mu}|\vec{k}+\vec{q}\rangle\rangle_c = c(t^{AA}-t^{BB})N\delta_{\vec{q}0}\nabla_{\vec{k}} s(\vec{k})$ not contributing to (11), because $\nabla_{\vec{k}} s(\vec{k})$ is an odd function of $\vec{k}$. Substituting (16) into (11) we find

$$\lim_{\omega\to 0} \tilde{\chi}_J^{+-}(\vec{q} = 0, \omega) = \frac{c\bar{U}}{12N}(t^{AA}-t^{BB})^2$$

$$\times \sum_{\vec{q}} \frac{\left| \frac{i}{N} \sum_{\vec{k}} \int \frac{dE}{2\pi} \mathcal{G}_{\vec{k}\uparrow}(E)\mathcal{G}_{\vec{k}+\vec{q}\downarrow}(E)\,(\nabla_{\vec{k}} s(\vec{k})+\nabla_{\vec{k}+\vec{q}} s(\vec{k}+\vec{q}))\right|^2}{1-\frac{\bar{U}_i}{N}\sum_{\vec{k}} \int \frac{dE}{2\pi}\mathcal{G}_{\vec{k}\uparrow}(E)\mathcal{G}_{\vec{k}+\vec{q}\downarrow}(E)}. \tag{17}$$

In the spin wave problem, we are interested in the magnon energy $\omega_q = Dq^2$ valid for small q. The spin wave stiffness constant D defined in general in [6] (cf. [3,7]) consists now of two terms

$$D = D_0 - \frac{1}{n_\uparrow - n_\downarrow} \lim_{\omega\to 0} \lim_{q\to 0} \tilde{\chi}_J^{+-}(\vec{q}, \omega) \tag{18}$$

corresponding to the so-called [2] average exchange and magnon scattering contributions. By taking into account CPA vertex corrections originated from off-diagonal disorder of the type (12), the explicit form of D_0 was derived to be [3]

$$D_0 = \frac{1}{6\pi(n_\uparrow - n_\downarrow)} \operatorname{Im} \int_{-\infty}^{\mu} dE[\Pi_{\uparrow\uparrow}(E^+, E^+) + \Pi_{\downarrow\downarrow}(E^+, E^+) - 2\Pi_{\uparrow\downarrow}(E^+, E^+)], \tag{19}$$

where

$$\Pi_{\sigma\sigma'}(z, z') = \frac{1}{N} \sum_{\vec{k}} \mathscr{G}_{\vec{k}\sigma}(z)\mathscr{G}_{\vec{k}\sigma'}(z') \left[\nabla_{\vec{k}}(t^{BB}s(\vec{k}) + \tfrac{1}{2}(\Sigma_\sigma(\vec{k}, z) + \Sigma_{\sigma'}(\vec{k}, z')))\right]^2$$

$$+ \frac{1}{N} \sum_{\vec{k}} [\sigma_{2\sigma}(z)\mathscr{G}_{\vec{k}\sigma'}(z') + \sigma_{2\sigma'}(z')\mathscr{G}_{\vec{k}\sigma}(z)] [\nabla_{\vec{k}} s(\vec{k})]^2. \tag{20}$$

The quantities involved in (19) and (20) are given below, and $E^+ = E + i0$. The second term of (18) is available from (17). It represents the vertex correction resulting from the interplay between interaction and off-diagonal disorder, provided that the spin wave is scattered by an inhomogeneous medium.

3. Computational method

The dynamics of the electron system in the ferromagnetic phase will be investigated in detail by an energy-dependent renormalization of the spin-band splitting. Adopting the CLA scheme [4] we can summarize the basic formulas as follows

$$\mathscr{G}_{\vec{k}\sigma}(z) = (z - \varepsilon^B - t^{BB}s(\vec{k}) - \Sigma_\sigma(\vec{k}, z))^{-1}, \tag{21}$$

$$\Sigma_\sigma(\vec{k}, z) = \sigma_{0\sigma}(z) + 2\sigma_{1\sigma}(z)s(\vec{k}) + \sigma_{2\sigma}(z)s^2(\vec{k}), \tag{22}$$

$$\langle \tau^\nu_{li\sigma}(z) \rangle_c = 0, \quad (l = 0, 1, 2) \tag{23}$$

$$\tilde{\varepsilon}^\nu_{i\sigma}(z) = \delta^\nu_i + \Sigma^\nu{}_{ii\sigma}(z); \quad \delta^\nu_i = \begin{cases} \varepsilon^A - \varepsilon^B, & \nu = A \\ 0, & \nu = B, \end{cases} \tag{24}$$

$$\Sigma^\nu_{Uii\sigma}(E) = \int \frac{dE'}{2\pi} G^\nu_{ii-\sigma}(E') T^\nu_i(E + E'), \quad (\nu = A, B) \tag{25}$$

$$T^\nu_i(E) = \left[\frac{1}{U^\nu_i} + \int \frac{dE'}{2\pi i} G^\nu_{ii\sigma}(E') G^\nu_{ii-\sigma}(E - E')\right]^{-1}, \tag{26}$$

$$G^\nu_{ii\sigma}(z) = F_{0\sigma}(z) + F^2_{0\sigma}(z)\tau^\nu_{0i\sigma}(z) + 2F_{0\sigma}(z)F_{1\sigma}(z)\tau^\nu_{1i\sigma}(z) + F^2_{1\sigma}(z)\tau^\nu_{2i\sigma}(z), \tag{27}$$

$$F_{l\sigma}(z) = \frac{1}{N} \sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z) \, [s(\vec{k})]^l, \tag{28}$$

$$n = \sum_{\sigma} n_\sigma = -\frac{1}{\pi} \sum_{\sigma} \int_{-\infty}^{\mu} dE \, \mathrm{Im} \, F_{0\sigma}(E^+). \tag{29}$$

Here we introduced the coherent self-energy $\Sigma_\sigma(\vec{k}, z)$, the one-particle scattering matrix parts $\tau^{\nu}_{ii\sigma}(z)$ given explicitly in [4], the correlation-conditioned self-energy $\Sigma^{\nu}_{Uii\sigma}(E)$, the two-particle T-matrix $T^{\nu}_i(E+E')$, the partially averaged Green function $G^{\nu}_{ii\sigma}(E)$, the average number of electrons per site (per site per spin) n (n_σ), and the Fermi energy μ. The functions $\sigma_{l\sigma}(z)$ are determined by the off-diagonal CPA coupled conditions (23), which contain the renormalized atomic potential $\tilde{\varepsilon}^{\nu}_{i\sigma}(z)$ (bare values are denoted by $\varepsilon^{\nu}_i = \varepsilon^{\nu}$).

To simplify matters, we choose the density of states and the mean-square velocity over a constant-energy surface related to the unperturbed pure B-band as

$$\frac{1}{N} \sum_{\vec{k}} \delta(E - \varepsilon^B_{\vec{k}}) = \frac{2}{\pi w^B} \left[1 - \left(\frac{E}{w^B}\right)^2\right]^{1/2} \theta(w^B - |E|), \tag{30}$$

$$\frac{1}{N} \sum_{\vec{k}} \delta(E - \varepsilon^B_{\vec{k}}) \, (\nabla_{\vec{k}} \varepsilon^B_{\vec{k}})^2 = \frac{2(v^B_m)^2}{\pi w^B} \left[1 - \left(\frac{E}{w^B}\right)^2\right]^{3/2} \theta(w^B - |E|), \tag{31}$$

where $\varepsilon^B_{\vec{k}} = t^{BB} s(\vec{k})$, $\varepsilon^B = 0$, $w^B = 6t^{BB}$ is the half-bandwidth within a sc n.n. model, and v^B_m is of order $w^B a$ (a — lattice constant). By means of (31) the $\vec{k}$-summation in (20) can be rewritten, using (21) and (22), in the form

$$\begin{aligned} \Pi_{\sigma\sigma'}(E^+, E^+) = \frac{2(v^B_m)^2}{\pi} \Bigg\{ \Bigg[1 + \frac{12}{w^B} (\sigma_{1\sigma}(E^+) + \sigma_{1\sigma'}(E^+)) + \frac{36}{(w^B)^2} (\sigma_{1\sigma}(E^+) \\ + \sigma_{1\sigma'}(E^+))^2 \Bigg] H_{0\sigma\sigma'}(E^+, E^+) + \frac{72}{w^B} (\sigma_{2\sigma}(E^+) + \sigma_{2\sigma'}(E^+)) \left(1 + \frac{6}{w^B} (\sigma_{1\sigma}(E^+) + \sigma_{1\sigma'}(E^+))\right) \\ \times H_{1\sigma\sigma'}(E^+, E^+) + \left[\frac{36}{w^B} (\sigma_{2\sigma}(E^+) + \sigma_{2\sigma'}(E^+))\right]^2 H_{2\sigma\sigma'}(E^+, E^+) \\ + \frac{36}{(w^B)^2} [\sigma_{2\sigma}(E^+) \hat{F}_{\sigma'}(E^+) + \sigma_{2\sigma'}(E^+) \hat{F}_{\sigma}(E^+)] \Bigg\}. \end{aligned} \tag{32}$$

The functions $H_{l\sigma\sigma'}(E^+, E^+)$ can be calculated by the residue method. Hence, in the spin-flip case, it results in

$$H_{0\uparrow\downarrow} = A(1 + w_{\uparrow 1} + w_{\uparrow 2} + w_{\downarrow 1} + w_{\downarrow 2}), \tag{33}$$

$$H_{1\uparrow\downarrow} = A(z_{\uparrow 1} + z_{\uparrow 2} + z_{\downarrow 1} + z_{\downarrow 2} + z_{\uparrow 1} w_{\uparrow 1} + z_{\uparrow 2} w_{\uparrow 2} + z_{\downarrow 1} w_{\downarrow 1} + z_{\downarrow 2} w_{\downarrow 2}), \tag{34}$$

$$\begin{aligned} H_{2\uparrow\downarrow} = A(z^2_{\uparrow 1} + z^2_{\uparrow 2} + z^2_{\downarrow 1} + z^2_{\downarrow 2} + z_{\uparrow 1} z_{\uparrow 2} + z_{\uparrow 1} z_{\downarrow 1} + z_{\uparrow 1} z_{\downarrow 2} + z_{\uparrow 2} z_{\downarrow 1} + z_{\uparrow 2} z_{\downarrow 2} \\ + z_{\downarrow 1} z_{\downarrow 2} + z^2_{\uparrow 1} w_{\uparrow 1} + z^2_{\uparrow 2} w_{\uparrow 2} + z^2_{\downarrow 1} w_{\downarrow 1} + z^2_{\downarrow 2} w_{\downarrow 2} - \tfrac{3}{2}) \end{aligned} \tag{35}$$

with

$$A = \frac{\pi}{36^2\sigma_{2\uparrow}(E^+)\sigma_{2\downarrow}(E^+)}, \quad w_{\uparrow 1} = \frac{i(1-z_{\uparrow 1}^2)\sqrt{1-z_{\uparrow 1}^2}}{(z_{\uparrow 1}-z_{\uparrow 2})(z_{\uparrow 1}-z_{\downarrow 1})(z_{\uparrow 1}-z_{\downarrow 2})}, \tag{36}$$

$$z_{\sigma 1,2} = -\frac{(w^B+12\sigma_{1\sigma})}{72\sigma_{2\sigma}} \pm \sqrt{\left(\frac{w^B+12\sigma_{1\sigma}}{72\sigma_{2\sigma}}\right)^2 + \frac{E^+-\sigma_{0\sigma}}{36\sigma_{2\sigma}}}, \tag{37}$$

where $w_{\uparrow 2}$ etc. are obtained by interchanging the labels, and $\sigma_{l\sigma} = \sigma_{l\sigma}(E^+)$. Besides, the analytical expressions of $H_{l\sigma\sigma}(E^+, E^+)$ and $\hat{F}_\sigma(E^+)$ are available from the conductivity treatment [5] by adding spin indices; $\hat{F}_\sigma(E^+)$ as well as $F_{l\sigma}(z)$ in (28) can be found analytically on the basis of (30).

4. Numerics and discussion

Now we compute self-consistent ferromagnetic solutions of the CLA scheme (21) to (29), completed by the assumption (30), for suitable values of the input parameters $w^A(=6t^{AA})$, w^B, ε^A, $U^\nu(=U_i^\nu)$, c, and n. The average electron number with spin σ at ν sites can be evaluated from

$$n_\sigma^\nu = \int_{-\infty}^{\mu} \varrho_\sigma^\nu(E)dE = -\frac{1}{\pi}\int_{-\infty}^{\mu} dE\, \mathrm{Im}\, G_{ii\sigma}^\nu(E^+), \quad (\nu = A, B) \tag{38}$$

where $\varrho_\sigma^\nu(E)$ is the partially averaged spin-dependent density of states.

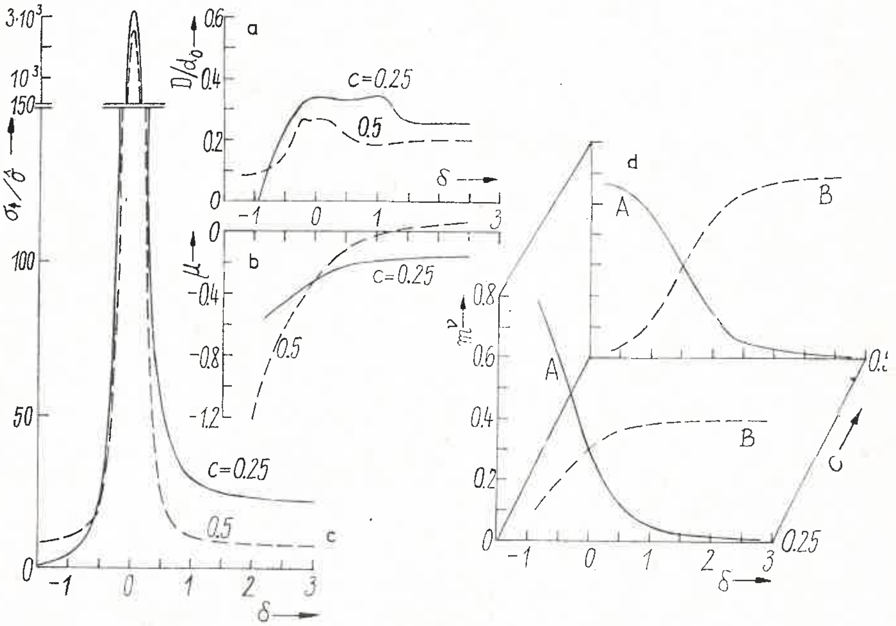

Fig. 1. a) Spin wave stiffness constant D, b) Fermi energy μ, c) dc conductivity $\sigma_\uparrow$, and d) partial magnetizations m^ν versus the scattering strength $\delta = \varepsilon^A - \varepsilon^B$ for two A_cB_{1-c} alloys with $(w, U^A, U^B, n) = (1, 2.5, 4.2, 0.3)$

The numerical example of Fig. 1 gives HFA results in the case of only diagonal disorder ($w^A = w^B = w$). This means that the self-energy $\Sigma_{Uii\sigma}^{\nu HF} = U^\nu n^\nu_{-\sigma}$ appears instead of (25) and (26), both $\sigma_{1\sigma}$ and $\sigma_{2\sigma}$ vanish. Fig. 1 shows the stiffness coefficient D in units of $d_0 = \frac{1}{9} wa^2$, the Fermi energy μ, the partial magnetizations $m^\nu = n^\nu_\uparrow - n^\nu_\downarrow$, and the spin up conductivity given at zero temperature by

$$\sigma_\uparrow = \hat{\sigma}\pi \left[(2(\text{Im}\, \sigma_{0\uparrow}(\mu^+))^2 + \frac{1}{\text{Im}\, \sigma_{0\uparrow}(\mu^+)} \text{Re}\, \{ i \sqrt{1-\hat{z}_\uparrow^2}\, (i(1-\hat{z}_\uparrow^2) + 3z_\uparrow \,\text{Im}\, \sigma_0\, (\mu^+)) \} \right], \quad (39)$$

where $\hat{z}_\uparrow = \mu^+ - \sigma_{0\uparrow}(\mu^+)$, and $\hat{\sigma} = e^2(v_m^B)^2 N/3\pi^2 V$[1]. Note that $\sigma_\downarrow = 0$ arises from the saturated magnetism. There $D > 0$ and $m > 0$ hold ($m = \langle m^\nu \rangle_c = cm^A + (1-c)m^B$), so that the criterion for stability of the ferromagnetic ground state against spin wave excitations is fulfilled.

In Figs 2–5 we are trying to model Pt_cNi_{1-c} alloys, as an appropriate object for CLA calculations in the presence of off-diagonal disorder, by adopting the pure values (cf. [8]) $(2w^{Pt}, 2w^{Ni}, \varepsilon^{Pt} - \varepsilon^{Ni}, U^{Pt}, U^{Ni}) = (7.8, 4.15, 0, 6.61, 14.11)$eV, and $n^{Pt} = 0.4$, $n^{Ni} = 0.6$ corresponding to the number of d-holes per atom. In alloying $n = cn^{Pt} + (1-c)n^{Ni}$ is fixed for a given concentration c.

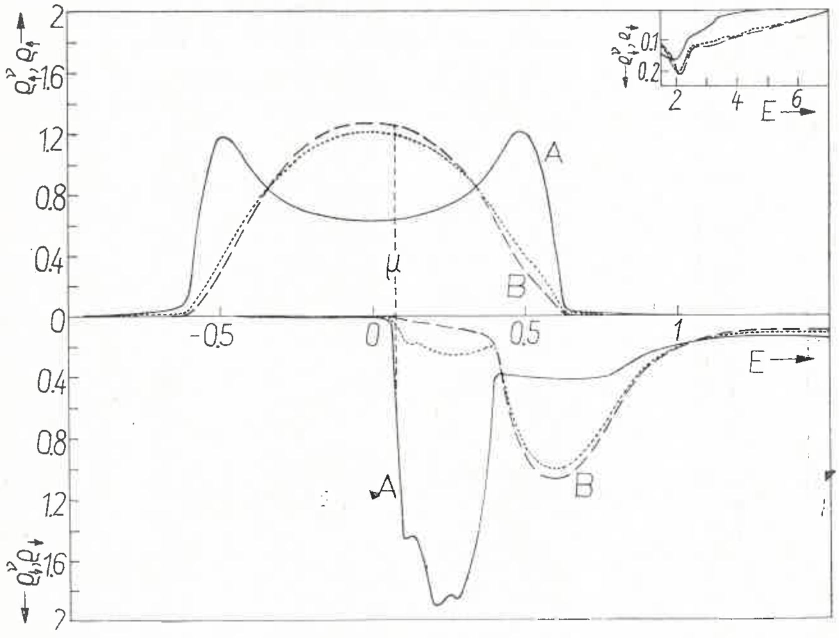

Fig. 2. Electron densities of states $\varrho^\nu_\sigma(E)$ ($\nu = A, B$) and $\varrho_\sigma(E)$, averaged partially and totally, resp., for an $A_{0.1}B_{0.9}$ alloy with the set $(2w^A, 2w^B, \varepsilon^A - \varepsilon^B, U^A, U^B) = (1.88, 1, 0, 1.59, 3.4)$

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[1] V is the volume of the system.

The calculated densities of states ϱ_σ^ν and $\varrho_\sigma = \langle \varrho_\sigma^\nu \rangle_c$ in Fig. 2 and Fig. 3 illustrate the variation of the spin band splitting with c in the case of off-diagonal disorder. The two-particle correlations provide large tails with small humps, especially for the minority spin (↓) electrons. According to the degree of saturation the shape of the spin ↑ band is weakly affected by correlations. In Fig. 3 and Fig. 4 we present at $c = 0.175$ in more detail the spectrum resulting from the self-consistent CLA computation. In this nearly saturated case the imaginary parts of the retarded self-energies $\sigma_{0\sigma}(E)$ and $\Sigma_{U\sigma}(E)$ indicate the distinct damping of the electron states with spin ↑ and ↓, because only electrons with antiparallel spins interact. Note that Fig. 4 exhibits, in units of $2w^B$, the retarded functions $\Sigma_{U\sigma}^\nu(E)$ and $T^\nu(E)$ ascribed to the causal functions in (25) and (26) (site index i is omitted). One sees that the effective local vertices $T^\nu(E)$ produce the damping effect on $\Sigma_{U\sigma}^\nu(E)$ and $\varrho_\sigma^\nu(E)$ in the two-particle region.

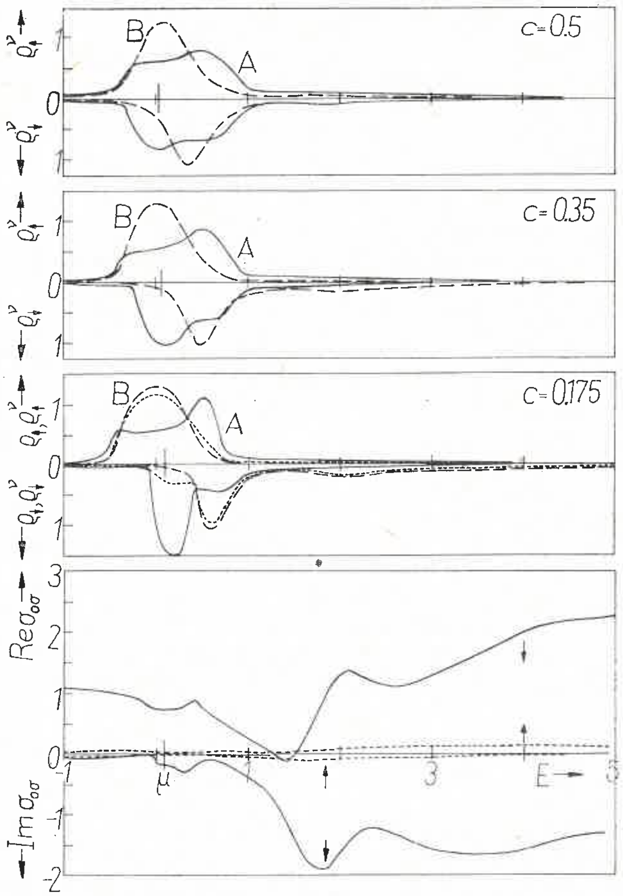

Fig. 3. Component densities of states $\varrho_\sigma^\nu(E)$ at various concentrations c; alloy density of states $\varrho_\sigma(E)$, real and imaginary parts of the coherent self-energy contribution $\sigma_{0\sigma}(E)$ at $c = 0.175$. The parameter set is the same as in Fig. 2

In Fig. 5a the reduced values of the effective Coulomb interaction $T^{\nu}(2\mu)$ are drawn as a function of composition of Pt_cNi_{1-c} alloys. The absolute values of $T^{\nu}(2\mu)$ decrease with c from 6.5 eV to 3 eV, i.e., the bare value U^{Ni} is diminished by a factor of about 4. The transition from ferromagnetism to paramagnetism connected with a critical concentration is pointed out by means of the stiffness coefficient D_0 (Fig. 5b) and the spin-dependent carrier densities n_{σ}^{ν} and n_{σ} (Fig. 5c). Contrary to the HFA values, the CLA results of D_0 in Fig. 5b show a peak at c_{cr} and refer to unstable ferromagnetic solutions for $c = 0.35$ and $c = 0.5$ in Fig. 3. A critical concentration of about $c_{cr} = 42$ at. % Ni in Pt is confirmed theoretically [8,9] and experimentally [10]. Note that correlations lead to $D_{Ni} = 558$ meVÅ² at $a = 3.8$ Å, whereas the HFA result for the same parameters is about two times greater.

In the numerical work only the average exchange stiffness D_0 was included. By taking into account the magnon scattering contribution (17) to (18) one may expect near c_{cr} a smaller D-maximum.

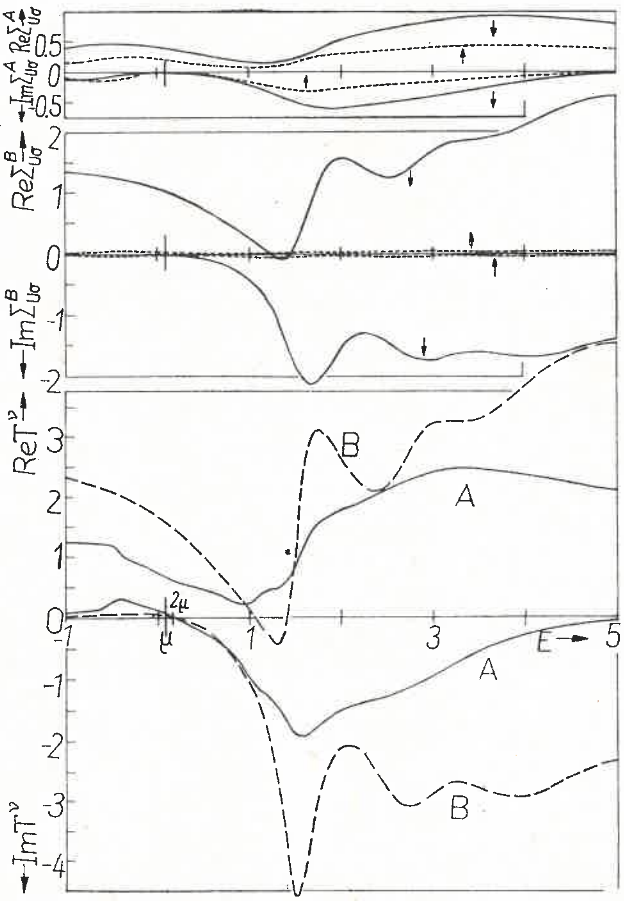

Fig. 4. Real and imaginary parts of the self-energies $\overset{\nu}{\Sigma}_{U\sigma}(E)$ and effective vertices $T^{\nu}(E)$ caused by electron-electron correlations; $c = 0.175$, the other parameters as in Fig. 2

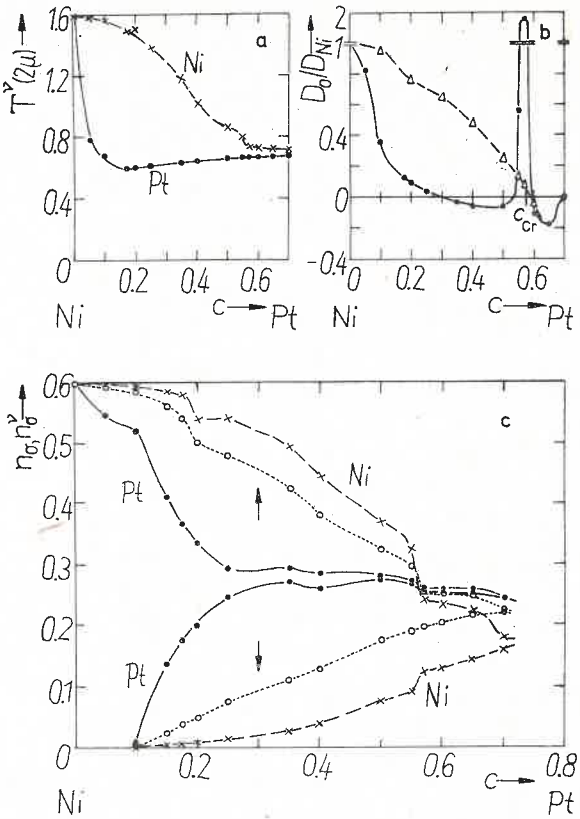

Fig. 5. a) Effective Coulomb interactions $T^{\nu}(2\mu)$, b) spin wave stiffness constant D_0 (●) compared with HFA results (Δ), c) partial and total carrier densities $\overset{\nu}{n}_{\sigma}$ and n_{σ}(○) versus c for Pt_cNi_{1-c} alloys corresponding to the parameter set in Fig. 2

Editorial note. This article was proofread by the editors only, not by the authors.

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