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Спиновые волны и их устойчивость в неупорядоченных ферромагнитных металлических сплавах

На основе микроскопической теории ферми-жидкости при нулевой температуре вычислена энергия длинноволновых спиновых возбуждений в ферромагнитных сплавах переходных металлов. В когерентном горизонтальном лестничном приближении для хаотической модели Хаббарда проведено самосогласованное вычисление перенормировки коэффициента жесткости D за счет электрон-электронных корреляций. Коэффициент D получен численным образом и используется для определения устойчивости ферромагнитного состояния. Полученные результаты сравниваются с экспериментальными данными по рассеянию нейтронов для сплавов на основе Ni.

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Ferromagnetic Spin Waves and Their Stability in Disordered Metallic Alloys

The energy of long-wavelength spin waves in ferromagnetic transition metal alloys is calculated within a microscopic Fermi liquid approach at zero temperature. The renormalization of the stiffness constant D due to electron-electron correlations is performed self-consistently in the coherent horizontal ladder approximation for the random Hubbard model. The stability of ferromagnetism is studied numerically in terms of D. A comparison with neutron scattering data for Ni -based alloys is given.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. INTRODUCTION

In itinerant-electron ferromagnets the stiffness constant D characterizes long-wavelength spin waves of the type $\omega_q = Dq^2$ below the Stoner gap in the particle-hole excitation spectrum. In particular, the stability of ferromagnetism in metallic systems, for instance in transition metal alloys, is related to the condition $D > 0$ provided that the magnetization is positive. Inelastic neutron scattering data of D for pure Ni [1] and Ni -based alloys (see, e.g., [2 to 5]) can be explained by an itinerant electron model. In the simplest version, the intra-atomic interaction between d-electrons produces the exchange splitting and their overlaps guarantee ferromagnetism.

The approach mostly used [6 to 10] to calculate D for alloys within a random version of the Hubbard model [11] is based on the random phase approximation (RPA), where the electron-electron interaction is taken into account in the Hartree-Fock (HF) approximation and the disorder in the coherent potential approximation (CPA) [12]. A RPA decoupling scheme was given in [13]. Beside CPA treatments there are rigid band calculations of D (cf. [5, 10]) in alloys performed with an adjusted band splitting depending on the impurity concentration.

In order to include electron correlation effects on D a theoretical scheme going beyond the RPA was proposed in [14], which is based on the coherent ladder approximation (CLA) [15,16], i.e., the self-consistent combination of the CPA and the local ladder approximation [17]

in the particle-particle channel. Such a T-matrix approximation is suitable for strong short-range interactions and low carrier densities, and can therefore be applied to Ni (0.6 holes per atom), Pd and Pt (0.4 holes per atom). The replacement of the energy-dependent T-matrix by an effective interaction of the Kanamori type [18], as used, e.g., in calculating the paramagnetic susceptibility [19] and the magnetostriction [20], leads again to a RPA-CPA treatment of spin waves.

In the present paper we calculate explicitly the stiffness constant D for disordered alloys within a microscopic Fermi liquid description [14] at zero temperature starting from a single-band random Hubbard model. The main features of this computation of D are as follows:

(i) Simplified assumptions on the pure unperturbed band permit one to carry out k-space integrations analytically.

(ii) Correlation effects are evaluated self-consistently from bare Coulomb interactions by retaining the energy-dependence of the T-matrices.

(iii) Weak and strong ferromagnetism are treated simultaneously. Numerical CLA results of D are compared with experimental values for NiFe and NiPd alloys. Moreover, the stability of ferromagnetism is also proved in terms of RPA-CPA solutions.

2. *STIFFNESS CONSTANT INCLUDING ELECTRON-ELECTRON CORRELATIONS*

It is satisfactory to base the ferromagnetism in narrow-band alloys A_cB_{1-c} on the Hubbard Hamiltonian [11] in the random form

$$H^{\{\nu\}} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} n_{\vec{k}\sigma} + \sum_{i\sigma} \epsilon_i^{\nu} n_{i\sigma} + \sum_i U_i^{\nu} n_{i\uparrow} n_{i\downarrow} , \qquad (1)$$

where $n_{\vec{k}\sigma}$ ($n_{i\sigma}$) is the occupation number operator for Bloch (Wannier) states with spin σ, and $\epsilon_{\vec{k}}$ is the band energy assumed to be independent of the atomic arrangement. Within the whole alloy configuration $\{\nu\}$ the

atomic energy ϵ_i^{ν} and the bare intra-atomic Coulomb interaction U_i^{ν} take the random values ϵ^{ν} and U^{ν} (ν=A,B), respectively, according to whether an A- or B-atom occupies the site i.

The spin wave energy $\omega_q = D q^2$ for cubic crystals can be determined by a pole of the transverse susceptibility $\chi^{+-}(\vec{q},\omega)$ giving rise to the spin wave stiffness constant

$$D = -\frac{1}{2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c} \lim_{\omega\to 0} \lim_{q\to 0} \left[\frac{\omega^2}{q^2}(\chi^{+-}(\vec{q},\omega) + \frac{2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c}{\omega})\right], \qquad (2)$$

where $2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c = (n_\uparrow - n_\downarrow)$ is the magnetization per site (n_σ: average number of σ electrons per site), $\langle\ldots\rangle^{\{\nu\}}$ means the ground-state expectation value within $\{\nu\}$, and $\langle\ldots\rangle_c$ denotes the configuration average. Alternatively, the formula

$$D = \frac{1}{2\langle\langle S_i^z\rangle^{\{\nu\}}\rangle_c} \left[\lim_{q\to 0} \frac{1}{q^2} \langle\langle [S_{\vec{q}}^{+}, qJ_{-\vec{q}}^{-}]\rangle^{\{\nu\}}\rangle_c - \lim_{\omega\to 0} \lim_{q\to 0} \chi_J^{+-}(\vec{q},\omega)\right] \qquad (3)$$

written down by means of the spin current-spin current response $\chi_J^{+-}(\vec{q},\omega)$ was applied to alloys in [7,10,13] (compare the derivation for pure systems [21]). For the model (1) the transverse spin density operator in the Fourier transform $S_{\vec{q}}^{+}$ (or $S_{-\vec{q}}^{-} = (S_{\vec{q}}^{+})^{+}$) and its current operator $J_{\vec{q}}^{+}$ (or $J_{-\vec{q}}^{-} = (J_{\vec{q}}^{+})^{+}$) being here nonrandom are given by

$$\left.\begin{aligned} S_{\vec{q}}^{+} &= \frac{1}{\sqrt{N}} \sum_{\vec{k}} c_{\vec{k}\uparrow}^{+} c_{\vec{k}+\vec{q}\downarrow} \\ q J_{\vec{q}}^{+} &= \frac{1}{\sqrt{N}} \sum_{\vec{k}} (\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}) c_{\vec{k}\uparrow}^{+} c_{\vec{k}+\vec{q}\downarrow} \end{aligned}\right\} \qquad (4)$$

where $c_{\vec{k}\sigma}^{+}$ ($c_{\vec{k}\sigma}$) creates (destroys) an electron in the state $|\vec{k}\sigma\rangle$, N is the number of lattice sites.

In the framework of a microscopic Fermi liquid description (cf. [14]) at zero temperature the susceptibilities in (2) and (3) can be expressed with (4) in terms of causal Green functions as follows:

$$\chi^{+-}(\vec{q},\omega) = -\langle\langle\langle S^{+}_{\vec{q}}, S^{-}_{-\vec{q}}\rangle\rangle\rangle^{\{\nu\}}_{\omega} \rangle_c = \frac{i}{N}\int\frac{dE}{2\pi} < \mathrm{tr}\{\Lambda^{\{\nu\}}_{0\uparrow_\downarrow}(E,E+\omega;\vec{q})\times$$

$$\times G^{\{\nu\}}_{\downarrow}(E+\omega)\lambda_0(-\vec{q})G^{\{\nu\}}_{\uparrow}(E)\}>_c , \qquad (5)$$

$$q^2\chi^{+-}_J(\vec{q},\omega) = -\langle\langle\langle q J^{+}_{\vec{q}}, qJ^{-}_{-\vec{q}}\rangle\rangle\rangle^{\{\nu\}}_{\omega}\rangle_c = \qquad (6)$$

$$= -\frac{i}{N}\int\frac{dE}{2\pi} < \mathrm{tr}\{\Lambda^{\{\nu\}}_{1\uparrow_\downarrow}(E,E+\omega;\vec{q})G^{\{\nu\}}_{\downarrow}(E+\omega)\lambda_1(-\vec{q})G^{\{\nu\}}_{\uparrow}(E)\}>_c ,$$

where

$$\Lambda^{\{\nu\}}_{\alpha ij}(E,E+\omega;\vec{q}) = \lambda_{\alpha ij}(\vec{q}) - \delta_{ij}\int\frac{d\bar{E}}{2\pi} i I^{\{\nu\}}_{i\ \uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;\omega)\times \qquad (7)$$

$$\times \sum_{mn} G^{\{\nu\}}_{im\uparrow}(\bar{E})\Lambda^{\{\nu\}}_{\alpha mn\ \uparrow\downarrow}(\bar{E},\bar{E}+\omega;\vec{q})G^{\{\nu\}}_{ni\downarrow}(\bar{E}+\omega); \quad (\alpha=0,1)$$

$$\left.\begin{aligned} \lambda_{0ij}(\vec{q}) &= e^{-i\vec{q}\vec{R}_i}\delta_{ij}, \quad \lambda_{1ij}(\vec{q}) = t_{ij}\,(e^{-i\vec{q}\vec{R}_i} - e^{-i\vec{q}\vec{R}_j}) \\ t_{ij} &= \frac{1}{N}\sum_{\vec{k}}\epsilon_{\vec{k}}\, e^{i\vec{k}(\vec{R}_i-\vec{R}_j)} \end{aligned}\right\} \qquad (8)$$

Here only the locality of the irreducible particle-hole vertex $I^{\{\nu\}}_{i\ \uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;\omega) \equiv I^{\{\nu\}}_{i\ \uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;E+\omega,\bar{E})$ has been assumed, and the trace means the summation (without spin) over one-particle states. The prescription (3) seems to be favoured instead of (2), because the Bethe-

Salpeter-type equation (7) for $\alpha=1$ can be solved without further assumptions on $I^{\{\nu\}}_{i\ \uparrow\downarrow\downarrow\uparrow}$. Then by expanding λ_1 and the effective spin-flip current $\Lambda^{\{\nu\}}_1$ in (6) and (7) to first order in $\vec{q}$ and employing the cubic symmetry in the following one gets

$$\chi^{+-}_J(\vec{q}=0,\omega) = \frac{i}{3N}\int\frac{dE}{2\pi} < \mathrm{tr}\{\vec{\Lambda}^{\{\nu\}}_{1\uparrow_\downarrow}(E,E+\omega)G^{\{\nu\}}_{\downarrow}(E+\omega)\vec{j}G^{\{\nu\}}_{\uparrow}(E)\}>_c , \qquad (9)$$

$$\vec{\Lambda}^{\{\nu\}}_{1\ ij\ \uparrow\downarrow}(E,E+\omega) = \vec{j}_{ij} - \delta_{ij}\int\frac{d\bar{E}}{2\pi} i I^{\{\nu\}}_{i\ \uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;\omega)\sum_{mn} G^{\{\nu\}}_{im\uparrow}(\bar{E})\times$$

$$\times \vec{\Lambda}^{\{\nu\}}_{1mn\ \uparrow\downarrow}(\bar{E},\bar{E}+\omega)G^{\{\nu\}}_{ni\downarrow}(\bar{E}+\omega); \qquad (10)$$

$$\vec{j}_{ij} = -it_{ij}(\vec{R}_i - \vec{R}_j),$$

where the notations $\lambda_1(\vec{q}) = \vec{q}\cdot\vec{j}$ and $\Lambda^{\{\nu\}}_{1\uparrow\downarrow}(E,E+\omega;\vec{q}) = \vec{q}\cdot\vec{\Lambda}^{\{\nu\}}_{1\uparrow\downarrow}(E,E+\omega)$ have been introduced ; under the trace $\vec{j}$ and $\vec{\Lambda}^{\{\nu\}}_1$ form a scalar product.

Separating diagonal and off-diagonal parts of $\vec{\Lambda}^{\{\nu\}}_1$ in (9) and (10) we obtain

$$\chi^{+-}_J(\vec{q}=0,\omega) = \frac{i}{3N}\int\frac{dE}{2\pi} < \mathrm{tr}\{\vec{j}G^{\{\nu\}}_{\downarrow}(E+\omega)\vec{j}\,G^{\{\nu\}}_{\uparrow}(E)\}>_c + \qquad (11)$$

$$+ \tilde{\chi}^{+-}_J(\vec{q}=0,\omega),$$

where

$$\tilde{\chi}^{+-}_J(\vec{q}=0,\omega) = \frac{i}{3N}\int\frac{dE}{2\pi} < \sum_i \vec{\Lambda}^{\{\nu\}}_{1\ ii\ \uparrow\downarrow}(E,E+\omega)\cdot\vec{K}^{\{\nu\}}_{ii\ \downarrow\uparrow}(E+\omega,E)>_c , \qquad (12)$$

$$\vec{K}^{\{\nu\}}_{ii\ \downarrow\uparrow}(E+\omega,E) = \sum_{mn} G^{\{\nu\}}_{im\downarrow}(E+\omega)\vec{j}_{mn}G^{\{\nu\}}_{ni\uparrow}(E). \qquad (13)$$

Since the configurational averaging in (12) is beyond the CPA we make the factorization ansatz [14] $<\vec{\Lambda}_1^{\{\nu\}} \cdot \vec{K}^{\{\nu\}}>_c = <\vec{\Lambda}_1^{\{\nu\}}>_c \cdot <\vec{K}^{\{\nu\}}>_c$ leading to

$$\vec{K}_{\downarrow\uparrow}(E+\omega, E) = < G_{\downarrow}^{\{\nu\}}(E+\omega)\vec{j}G_{\uparrow}^{\{\nu\}}(E)>_{cii} = \frac{1}{N}\sum_{\vec{k}} \mathcal{G}_{\vec{k}\downarrow}(E+\omega)\mathcal{G}_{\vec{k}\uparrow}(E)\, V_{\vec{k}\epsilon_{\vec{k}}} = 0 \qquad (14)$$

and $\tilde{\chi}_J^{+-}(\vec{q}=0,\omega) = 0$ due to time-reversal symmetry. $\mathcal{G}_{\vec{k}\sigma}$ denotes the coherent one-particle Green function including electron-electron correlations (see below). Thus we are left with the CPA result without vertex corrections, i.e.,

$$\chi_J^{+-}(\vec{q}=0,\omega) = \frac{i}{3N}\int \frac{dE}{2\pi}\sum_{\vec{k}} \mathcal{G}_{\vec{k}\downarrow}(E+\omega)\mathcal{G}_{\vec{k}\uparrow}(E)(V_{\vec{k}\epsilon_{\vec{k}}})^2. \qquad (15)$$

Substituting (15) and

$$\lim_{q\to 0}\frac{1}{q^2} <<[S_{\vec{q}}^{+}, qJ_{-\vec{q}}^{-}]>^{\{\nu\}}>_c = \frac{1}{6N}\sum_{\vec{k}\sigma} <<n_{\vec{k}\sigma}>^{\{\nu\}}>_c V_{\vec{k}\epsilon_{\vec{k}}}^2 \qquad (16)$$

into (3) and going over from the causal to retarded ("r") Green functions one finds

$$D = \frac{1}{6\pi(n_{\uparrow}-n_{\downarrow})}\,\mathrm{Im}\int_{-\infty}^{\mu} dE\,\frac{1}{N}\sum_{\vec{k}}(\mathcal{G}_{\vec{k}\uparrow}^{r}(E)-\mathcal{G}_{\vec{k}\downarrow}^{r}(E))^2 (V_{\vec{k}\epsilon_{\vec{k}}})^2, \qquad (17)$$

where μ is the Fermi energy. This expression for D agrees formally with the RPA-CPA result [6,7,10], which was based on the HF treatment of the electron-electron interaction.

In the present calculation, however, $\mathcal{G}_{\vec{k}\sigma}$ is dressed in the CLA scheme [16]. Then the correlation part expressed in terms of partially averaged causal functions reads

$$\Sigma_{Uii\sigma}^{\nu}(E) = \int \frac{d\bar{E}}{2\pi i} G_{ii-\sigma}^{\nu}(\bar{E}) T_i^{\nu}(E+\bar{E}), \qquad (\nu = A, B), \qquad (18)$$

$$T_i^{\nu}(E) = \left[\frac{1}{U_i^{\nu}} + \int \frac{d\bar{E}}{2\pi i} G_{ii\sigma}^{\nu}(\bar{E}) G_{ii-\sigma}^{\nu}(E-\bar{E})\right]^{-1}, \qquad (19)$$

where T_i^{ν} is the effective two-particle vertex. The local Green function $G_{ii\sigma}^{\nu}(z)$ written as resolvent (z being the complex energy) is renormalized by

$$G_{ii\sigma}^{\nu}(z) = \frac{F_\sigma(z)}{1-(\tilde{\epsilon}_{i\sigma}^{\nu}(z)-\Sigma_\sigma(z))F_\sigma(z)}, \qquad (20)$$

$$\tilde{\epsilon}_{i\sigma}^{\nu}(z) = \epsilon_i^{\nu} + \Sigma_{Uii\sigma}^{\nu}(z), \qquad (21)$$

$$F_\sigma(z) = \frac{1}{N}\sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z), \qquad (22)$$

$$\mathcal{G}_{\vec{k}\sigma}(z) = (z-\epsilon_{\vec{k}}-\Sigma_\sigma(z))^{-1}, \qquad (23)$$

$$\Sigma_\sigma(z) = c\tilde{\epsilon}_\sigma^{A}(z) + (1-c)\tilde{\epsilon}_\sigma^{B}(z) - [\tilde{\epsilon}_\sigma^{A}(z)-\Sigma_\sigma(z)]F_\sigma(z)[\tilde{\epsilon}_\sigma^{B}(z)-\Sigma_\sigma(z)], \qquad (24)$$

$$n = \sum_\sigma n_\sigma = -\frac{1}{\pi}\sum_\sigma \int_{-\infty}^{\mu} dE\,\mathrm{Im}\,F_\sigma^{r}(E). \qquad (25)$$

Here Σ_σ is the coherent potential, n is the average number of electrons per site. Contrary to the usual CPA [12], the atomic potential $\tilde{\epsilon}_{i\sigma}^{\nu}(z)$ (i is dropped in (24)) becomes energy-dependent through the self-energy $\Sigma_{Uii\sigma}^{\nu}(z)$ caused by correlations.

In the HF approximation the modified CPA problem (20) to (25) must be completed only, instead of (18) and (19), by the constant self-energy $\Sigma_{Uii\sigma}^{\nu HF} = U_i^{\nu} n_{i-\sigma}^{\nu}$, where $n_{i\sigma}^{\nu}$ is the average electron number with spin σ at ν sites given by

$$n_{i\sigma}^{\nu} = -\frac{1}{\pi}\int_{-\infty}^{\mu} dE\,\mathrm{Im}\,G_{ii\sigma}^{r\nu}(E). \qquad (26)$$

Taking into account the special vertex $I^{\{\nu\}}_{i\ \uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;\omega) = -T^{\{\nu\}}_{i\ \uparrow\downarrow\uparrow\downarrow}(E+\bar{E}+\omega) \equiv -T^{\{\nu\}}_{i}(E+\bar{E}+\omega)$, the equations (7), (18) and (19) with ν replaced by $\{\nu\}$ yield the identity [14]

$$\omega\,\Lambda^{\{\nu\}}_{0i\ \uparrow\downarrow}(E,E+\omega;\vec{q})\delta_{ij} - \Lambda^{\{\nu\}}_{1ij\ \uparrow\downarrow}(E,E+\omega;\vec{q}) = e^{-i\vec{q}\vec{R}_i}\,G^{\{\nu\}-1}_{ij\downarrow}(E+\omega) - G^{\{\nu\}-1}_{ij\uparrow}(E)\,e^{-i\vec{q}\vec{R}_j}, \tag{27}$$

with

$$(G^{\{\nu\}-1}(E))_{ij\sigma} = (E-\epsilon^{\nu}_{i})\delta_{ij} - t_{ij} - \Sigma^{\{\nu\}}_{Uii\sigma}(E)\delta_{ij}, \tag{28}$$

where the site-diagonality of $\Lambda^{\{\nu\}}_{0ij\ \uparrow\downarrow} = \Lambda^{\{\nu\}}_{0i\ \uparrow\downarrow}\delta_{ij}$ has been used in (27). Hence, in the completely random version $\{\nu\}$, the local ladder approximation fulfils the Ward-Takahashi-type relation (27).

The stability condition of the ferromagnetic ground state against spin wave excitations

$$\hat{D} = D(n_{\uparrow}-n_{\downarrow}) > 0 \tag{29}$$

may be found from the spectral representation

$$\chi^{+-r}(\vec{q},\omega) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega'\,\frac{\mathrm{sign}\,\omega'}{\omega-\omega'+i\epsilon}\,\hat{I}_{S^{+}_{\vec{q}}S^{-}_{-\vec{q}}}(\omega'), \tag{30}$$

where the spectral density $\hat{I}_{S^{+}_{\vec{q}}S^{-}_{-\vec{q}}}(\omega) \geq 0$ is related to a configurationally averaged system. The magnon pole

$$\chi^{+-r}_{\mathrm{pole}}(\vec{q},\omega) = -\frac{n_{\uparrow}-n_{\downarrow}}{\omega - Dq^2 + i\epsilon} \tag{31}$$

can be separated for small q and ω (Goldstone theorem) from the Stoner continuum, since the individual excitations have vanishing spectral weight for $\vec{q}\to 0$. In (31) the damping is omitted, and the residue is written down only in the lowest order of q. The comparison of (30) and (31) leads to (29) [14].

In the present approximation the spin wave damping γ_q entering into (31) instead of ϵ can be proved to be

$$\gamma_q = \frac{q^2}{n_{\uparrow}-n_{\downarrow}}\,\mathrm{Im}\chi^{+-r}_{J}(0,Dq^2) = \frac{Dq^4}{3\pi(n_{\uparrow}-n_{\downarrow})N}\sum_{\vec{k}}\mathrm{Im}\mathcal{G}^{r}_{\vec{k}\uparrow}(\mu)\,\mathrm{Im}\mathcal{G}^{r}_{\vec{k}\downarrow}(\mu)\,(\nabla_{\vec{k}}\epsilon_{\vec{k}})^2, \tag{32}$$

taking the same form as in RPA-CPA [8]; however, here electron-electron scatterings are included.

3. *NUMERICAL ANALYSIS AND CONCLUSION*

To carry out part of the computation of D analytically we choose simplified expressions [22] for the unperturbed density of states (per site per spin) $\rho_0(E)$ and the mean-square velocity over a constant-energy surface as follows:

$$\rho_0(E) = \frac{1}{N}\sum_{\vec{k}}\delta(E-\epsilon_{\vec{k}}) = \frac{2}{\pi w}\left[1-\left(\frac{E}{w}\right)^2\right]^{1/2}\theta(w-|E|), \tag{33}$$

$$\frac{1}{N}\sum_{\vec{k}}\delta(E-\epsilon_{\vec{k}})(\nabla_{\vec{k}}\epsilon_{\vec{k}})^2 = \frac{2v_m^2}{\pi w}\left[1-\left(\frac{E}{w}\right)^2\right]^{3/2}\theta(w-|E|), \tag{34}$$

where w is the half bandwidth, and v_m is of order wa with a being the lattice spacing. By means of (33) the $\vec{k}$-summation in (22) yields

$$F_{\sigma}(z) = \frac{2}{w}(\tilde{z}_{\sigma} - i\sqrt{1-\tilde{z}^2_{\sigma}}), \qquad \tilde{z}_{\sigma} = \frac{z-\Sigma_{\sigma}(z)}{w}. \tag{35}$$

To make (35) univalent we take that branch in the $\tilde{z}_\sigma$-plane with a cut along the real axis from -1 to 1, where the square root is positive on the upper lip of the cut.

Rewriting (17) as

$$D = \frac{1}{6\pi(n_\uparrow - n_\downarrow)} \mathrm{Im} \int_{-\infty}^{\mu} dE\, [\Pi^{rr}_{\uparrow\uparrow}(E,E) + \Pi^{rr}_{\downarrow\downarrow}(E,E) - 2\Pi^{rr}_{\uparrow\downarrow}(E,E)] \quad (36)$$

with the abbreviations $\Pi^{rr}_{\sigma\sigma'}(E,E) \equiv \Pi_{\sigma\sigma'}(E^+,E^+), E^+ = E+i0$, and

$$\Pi_{\sigma\sigma'}(z,z') = \frac{1}{N} \sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z) \mathcal{G}_{\vec{k}\sigma'}(z') (V_{\vec{k}} \epsilon_{\vec{k}})^2 \quad (37)$$

we find in performing the $\vec{k}$-sum with (34) by the residue method the current polatization parts

$$\Pi^{rr}_{\sigma\sigma} = \frac{2v_m^2}{w^2} (3z_\sigma^2 - \frac{3}{2} - 3iz_\sigma \sqrt{1-z_\sigma^2}), \quad z_\sigma = \frac{E^+ - \Sigma_\sigma(E^+)}{w}, \quad (38)$$

$$\Pi^{rr}_{\uparrow\downarrow} = \frac{2v_m^2}{w^2} (z_\uparrow^2 + z_\downarrow^2 + z_\uparrow z_\downarrow - \frac{3}{2} + i \frac{(1-z_\uparrow^2)^{3/2} - (1-z_\downarrow^2)^{3/2}}{z_\uparrow - z_\downarrow}). \quad (39)$$

From (36), (38), and (39) it results

$$D = \frac{v_m^2}{3\pi w^2 (n_\uparrow - n_\downarrow)} \mathrm{Im} \int_{-\infty}^{\mu} dE\, [(z_\uparrow - z_\downarrow)^2 - i\sqrt{1-z_\uparrow^2}(3z_\uparrow + \frac{2(1-z_\uparrow^2)}{z_\uparrow - z_\downarrow}) -$$
$$- i\sqrt{1-z_\downarrow^2}(3z_\downarrow - \frac{2(1-z_\downarrow^2)}{z_\uparrow - z_\downarrow})], \quad (40)$$

where the complex square roots are taken in the sense mentioned above.

The scalar dc conductivity σ at zero temperature can be calculated with the "same accuracy" as D. This leads to the modified Kubo-Greenwood formula

$$\sigma = \frac{e^2 N}{6\pi V} \sum_\sigma [\Pi^{ra}_{\sigma\sigma}(\mu,\mu) - \mathrm{Re}\,\Pi^{rr}_{\sigma\sigma}(\mu,\mu)] \equiv \sum_\sigma \sigma_\sigma \quad (41)$$

including Green functions renormalized by electron correlations within the CLA. Here $\Pi^{ra}_{\sigma\sigma}(\mu,\mu) \equiv \Pi_{\sigma\sigma}(\mu^+,\mu^-)$, $\mu^- = \mu - i0$, V is the volume of the system, and e is the unit charge. By inserting (38) and (39) with the replacement $\Pi^{ra}_{\sigma\sigma} = \Pi^{rr}_{\uparrow\downarrow}[z_\uparrow \to \hat{z}_\sigma, z_\downarrow \to \hat{z}^*_\sigma]$ into (41) we get the spin-dependent dc conductivity (for $\mathrm{Im}\,\Sigma_\sigma(\mu^+) < 0$)

$$\sigma_\sigma = \hat{\sigma}\pi [\frac{2(\mathrm{Im}\,\Sigma_\sigma(\mu^+))^2}{w^2} + \frac{w}{\mathrm{Im}\,\Sigma_\sigma(\mu^+)} \mathrm{Re}\{i\sqrt{1-\hat{z}_\sigma^2}(i(1-\hat{z}_\sigma^2) +$$
$$+ \frac{3}{w} \hat{z}_\sigma \mathrm{Im}\,\Sigma_\sigma(\mu^+))\}], \quad (42)$$

where

$$\hat{z}_\sigma = \frac{\mu^+ - \Sigma_\sigma(\mu^+)}{w}, \quad \hat{\sigma} = \frac{e^2 v_m^2 N}{3\pi^2 V}. \quad (43)$$

The numerical analysis is performed as follows: Choose the parameters $w, \epsilon^A, \epsilon^B = 0$ fixed, U^A, U^B, c, and n; solve the self-consistency loop (18) to (25) with the explicit Green function (35), and use these results to obtain D from (40) via the E-integration.

Figure 1 shows the transition region between weak and strong ferromagnetism versus the strengths of the intra-atomic Coulomb repulsion U^ν treated here in the HF approximation. In particular, the sets with $U^A = 2$, $U^B = 0$ and $U^A = 2$, $U^B = 2$ have been investigated in [23], but not in the context of spin waves. The RPA-CPA results (a) for the stiffness constant D (in units of $d_0 = \frac{1}{9} w a^2$) refer to the instability of the ferromagnetic ground state against spin wave excitations. Note that a crossing of the spin-dependent dc conductivities σ_σ(b) is found (cf. [24]). The component and average magnetizations $m^\nu = n^\nu_\uparrow - n^\nu_\downarrow$ and $m = n_\uparrow - n_\downarrow$, resp., are drawn in *Fig. 1d*.

Figure 2 represents a confined region of stable (mainly saturated) ferromagnetism ($D > 0$ (b), $m^\nu > 0$ (a)) depending on the electron density n. The zero of D at

the lower value of n corresponds roughly to a Stoner-like criterion (cf./16/), while the other zero signals

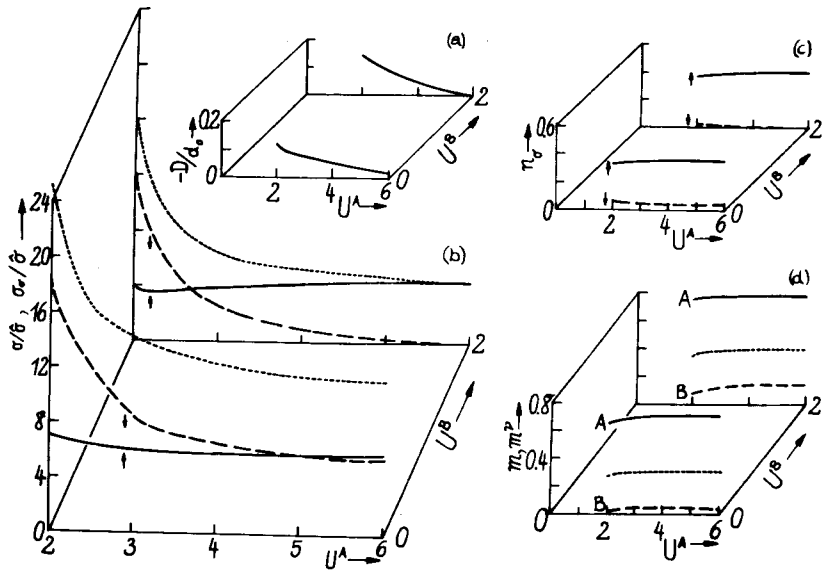

Fig. 1. a) Unstable ferromagnetism characterized by the spin wave stiffness constant $D<0$, *b)* dc *conductivities* σ_σ *and* σ, *c) electron densities* n_σ, *and d) magnetizations* m^ν *and* m *versus* U^ν *for an alloy with* $(w, \epsilon^A, \epsilon^B, c, n) = (1, -0.8, 0, 0.4, 0.4)$. *Hartree-Fock treatment of the electron-electron interaction.*

a change of the spin arrangement. Note that the maxima of D and $\sigma_\uparrow$(d) occur nearly at the same n values.

Most of the data on the stiffness constant D exist for NiFe alloys as reported in *Fig. 3*. As a test, we have taken into account electron-electron correlations, although the present scheme is more suited to describe the nickel component with 0.6 holes per atom in the d band than the iron component with a high local hole density. In *Fig. 3* the D values (x) calculated on the basis of the CLA are compared with (a) results obtained in RPA-CPA /7,9/, "rigid band" theory /10/, in the approach /13/, and with inelastic neutron scattering data /1,2,3/. The small value of D at $c = 0.4$ (b) shows

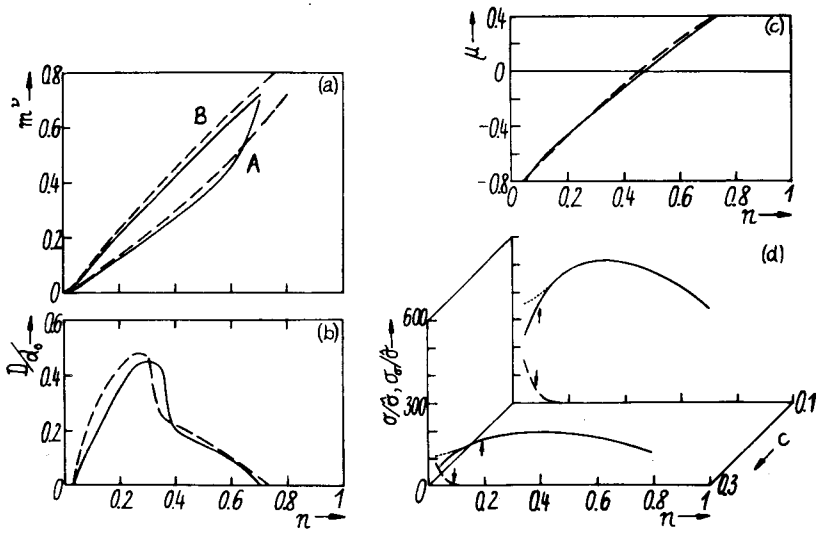

Fig. 2. a) Partial magnetizations m^ν, *b) spin wave stiffness constant* D *in the stable ferromagnetic case, c) Fermi energy* μ, *and d)* dc *conductivities* σ_σ *and* σ *versus* n *at the alloy concentrations* $c = 0.1$ *(full lines in a), b), c)) and* $c = 0.3$ *(dashed lines in a), b), c)) for the set* $(w, \epsilon^A, \epsilon^B, U^A, U^B) = (1, 0.2, 0, 4, 3)$. *Hartree-Fock treatment of the electron-electron interaction.*

that our model calculation can be justified only for small Fe concentrations. Note that for pure Ni the stiffness constant is found close to $D_{Ni} = 555$ *meV* Å^2 measured at 4.2 *K* /1/.

Electron correlation effects on the stiffness constant D in NiPd alloys are studied in *Fig. 4*, and a comparison with /25/ is given. This material is a good candidate for the CLA due to the small density of holes. For the pure systems the parameters are chosen as proposed in /20/; in alloying one has $n = cn^{Pd} + (1-c)n^{Ni}$, and the different hopping integrals are taken into account by putting the bandwidth $2w = c(2w)^{Pd} + (1-c)(2w)^{Ni}$. Note that in reduced units U^{Pd}, U^{Ni}, $\epsilon^{Pd} - \epsilon^{Ni}$ are scaled for all c by $2w = 1$. The bare U^ν are dressed self-consistently yielding the two-particle vertices $T_i^\nu(E+\bar{E})$,

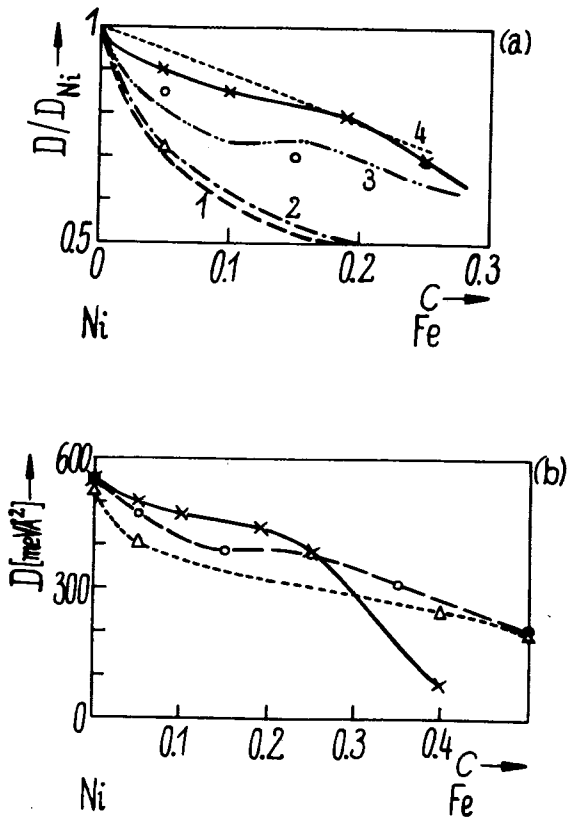

Fig. 3. Spin wave stiffness constant D *versus* c *for* Fe_cNi_{1-c} *alloys.* D *values (x) based on the coherent ladder approximation with* $(w, \epsilon^A, \epsilon^B, U^A, U^B, n_c) =$ *=(0.5, -0.24, 0, 2.66, 3.4, 0.6) (*$2w = 4.15$ *eV,* $a = 4$ Å *in absolute units in b)). Comparison with a) results computed in* [7] *(1),* [9] *(2),* [10] *(3),* [13] *(4) and a), b) experimental data given in* [1] *(□),* [2] *(Δ),* [3] *(○).*

especially $\Gamma^\nu = T_i^\nu(2\mu)$ and $\Gamma = c\Gamma^A + (1-c)\Gamma^B$ are plotted in reduced units in *Fig. 4d.*

The numerical results of the present model calculation exhibit the marked influence of the electron-electron correlations on the magnon energy in the long-wavelength limit $\omega_q = Dq^2$. Although a single-band Hubbard model with simplified band structure and diagonal dis-

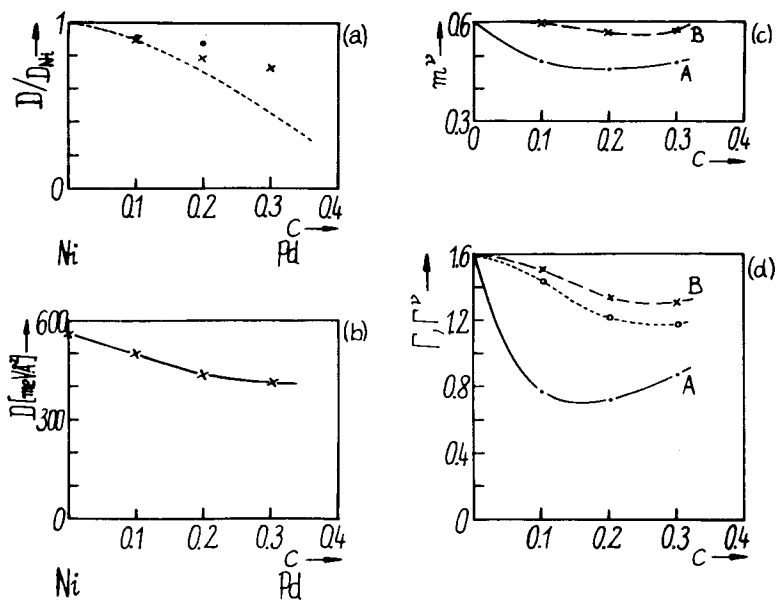

Fig. 4. Pd_cNi_{1-c} *alloys treated by using the coherent ladder approximation with the set* $((2w)^{Pd}, (2w)^{Ni}$ $\epsilon^{Pd} - \epsilon^{Ni}, U^{Pd}, U^{Ni}, n^{Pd}, n^{Ni}) =$ *(6.05 eV, 4.15 eV, 0.3 eV, 9.17 eV, 14.11 eV, 0.4, 0.6). a) Stiffness constant* D *values (x) compared with results in* [25] *(- - -) and experimental points (●) quoted in* [25]*, b)* D *in absolute units* (a=3.8 Å)*, c) partial magnetizations* m^ν*, and d) effective Coulomb interactions* Γ^ν *and* Γ *versus* c.

order only is taken into account, physically reasonable D values are found for Ni-based alloys. Beyond the RPA-CPA treatment, the approach given here is based on the coherent horizontal ladder approximation. Locality of the energy-dependent two-particle vertices is assumed which allows to preserve the single-site character of the CPA. The spin wave damping is proved to be small at least of order q^4. Thus a practicable method is proposed which retains the self-consistency to find stable ferromagnetism in transition metal alloys.

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