E. Kolley, W. Kolley, A. L. Kuzemsky

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AND THEIR STABILITY
IN DISORDERED METALLIC ALLOYS

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Kolley E., Kolley W., Kuzemsky A.L.

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.

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1. INTRODUCTION

In itinerant-electron ferromagnets the stiffness constant $D$ characterizes long-wavelength spin waves of the type $\omega_q = D q^2$ 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\textsuperscript{1}/ and Ni-based alloys (see, e.g.,\textsuperscript{2} to \textsuperscript{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 to calculate $D$ for alloys within a random version of the Hubbard model\textsuperscript{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)\textsuperscript{12}. A RPA decoupling scheme was given in\textsuperscript{13}. Beside CPA treatments there are rigid band calculations of $D$ (cf.\textsuperscript{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\textsuperscript{14}, which is based on the coherent ladder approximation (CLA)\textsuperscript{15,16}, i.e., the self-consistent combination of the CPA and the local ladder approximation\textsuperscript{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\textsuperscript{1181}, as used, e.g., in calculating the paramagnetic susceptibility\textsuperscript{1191} and the magnetostriction\textsuperscript{1201}, 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\textsuperscript{1141} 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 $A_{c}B_{1-c}$ on the Hubbard Hamiltonian\textsuperscript{111} in the random form

$$H = \sum_{\nu} \epsilon_{\nu} n_{\nu} + \sum_{\sigma} \epsilon_{\sigma} n_{\sigma} + \sum_{\nu} U_{\nu} n_{\nu} n_{\nu+1}$$

where $n_{\sigma}$ ($n_{\nu}$) is the occupation number operator for Bloch (Wannier) states with spin $\sigma$, and $\epsilon_{\nu}$ is the band energy assumed to be independent of the atomic arrangement. Within the whole alloy configuration $|\nu|$ the atomic energy $\epsilon_{\nu}$ and the bare intra-atomic Coulomb interaction $U_{\nu}$ take the random values $\epsilon_{\nu}$ and $U_{\nu}$, respectively, according to whether an $A$- or $B$-atom occupies the site $\nu$.

The spin wave energy $\omega_{q} = D q^{2}$ for cubic crystals can be determined by a pole of the transverse susceptibility $\chi_{\nu}^{\perp}(q,\omega)$ giving rise to the spin wave stiffness constant

$$D = \frac{1}{2 \langle S_{i} \rangle_{i}} \lim_{\omega \to 0, q \to 0} \langle S_{i} \rangle_{i} \chi_{\nu}^{\perp}(q,\omega)$$

where $2 \langle S_{i} \rangle_{i}$ is the magnetization per site ($n_{\sigma}$: average number of $\sigma$ electrons per site), $\langle ... \rangle_{i}$ means the ground-state expectation value within $|\nu\rangle$, and $\langle ... \rangle_{=}$ denotes the configuration average. Alternatively, the formula

$$D = \frac{1}{2 \langle S_{i} \rangle_{i}} \lim_{\omega \to 0, q \to 0} \langle S_{i} \rangle_{i} \chi_{\nu}^{\perp}(q,\omega)$

written down by means of the spin current-spin current response $\chi_{\nu}^{\perp}(q,\omega)$ was applied to alloys in\textsuperscript{17,10,131} (compare the derivation for pure systems\textsuperscript{21}). For the model (1) the transverse spin density operator in the Fourier transform $S_{q}^{+}$ (or $S_{-q}^{-}$) and its current operator $J_{q}^{\perp}$ (or $J_{-q}^{-}$) being here nonrandom are given by

$$S_{q}^{+} = \frac{1}{\sqrt{N}} \sum_{k} c^{+}_{k+q_{i}} c_{k+q_{i}}$$

$$J_{q}^{\perp} = \frac{1}{\sqrt{N}} \sum_{k} (\epsilon_{k+q_{i}} - \epsilon_{k}) c^{+}_{k+q_{i}} c_{k+q_{i}}$$

where $c^{+}_{k\sigma}$ ($c_{k\sigma}$) creates (destroys) an electron in the state $|k\sigma\rangle$. $N$ 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:

\[
\chi^+(q,\omega) = \frac{1}{N} \int \frac{dE}{2\pi} \text{tr} \left[ \Lambda_0^{[\nu]} (E, E+\omega; \bar{q}) \times \right.
\]
\[
G_{\downarrow}^{[\nu]} (E+\omega) \lambda_0^{(-\bar{q})} G_{\uparrow}^{[\nu]} (E) \bigg|_c,
\]

\[
q^0 \chi^{+}_J (q,\omega) = \frac{1}{N} \int \frac{dE}{2\pi} \text{tr} \left[ \Lambda_1^{[\nu]} (E, E+\omega; \bar{q}) G_{\downarrow}^{[\nu]} (E+\omega) \lambda_1^{(-\bar{q})} G_{\uparrow}^{[\nu]} (E) \bigg|_c,
\]

where

\[
\Lambda_1^{[\nu]} (E, E+\omega; \bar{q}) = \lambda_{0_{ij}} (\bar{q}) - \delta_{ij} \int \frac{dE}{2\pi} iI_1^{[\nu]} (E, E+\omega; \bar{q}) \times
\]
\[
\sum_{m_n} G_{im+}^{[\nu]} (E) A_{amn}^{[\nu]} (E, E+\omega; \bar{q}) G_{ni+}^{[\nu]} (E+\omega); \quad (a = 0, 1)
\]

\[
\lambda_0^{[\nu]} (\bar{q}) = e^{-i\bar{q} \vec{R}_{ij}}, \quad \lambda_1^{[\nu]} (\bar{q}) = t_{ij} (e^{-i\bar{q} \vec{R}_{ij}} - 1)
\]

\[
t_{ij} = \frac{1}{N} \sum_k \epsilon_k \epsilon_{\bar{k}} e^{ik \vec{R}_i - (\bar{k} \vec{R}_j)}
\]

Here only the locality of the irreducible particle-hole vertex \( I_1^{[\nu]} (E, E+\omega; \omega) \equiv I_1^{[\nu]} (E, E+\omega; E+\omega, E) \) 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 \( \nu = 1 \) can be solved without further assumptions on \( I_1^{[\nu]} \). Then by expanding \( \lambda_1^{[\nu]} \) and the effective spin-flip \( \Lambda_1^{[\nu]} \) in (6) and (7) to first order in \( \bar{q} \) and employing the cubic symmetry in the following one gets

\[
\chi^+_{J\downarrow} (q = 0, \omega) = \frac{1}{3N} \int \frac{dE}{2\pi} \text{tr} \left[ \sum_{m_n} I_1^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{im+}^{[\nu]} (E+\omega) \right. \]
\[
\times \Lambda_{1i}^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{ni+}^{[\nu]} (E+\omega),
\]

\[
+ \sum_{m_n} I_1^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{im+}^{[\nu]} (E+\omega) \Lambda_{1i}^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{ni+}^{[\nu]} (E+\omega),
\]

(12)

where the notations \( \lambda_1^{[\nu]} = q \downarrow \bar{q} \uparrow, \quad \lambda_1^{[\nu]} = q \uparrow \bar{q} \uparrow \) have been introduced; under the trace \( \sum_{m_n} I_1^{[\nu]} \) and \( \Lambda_1^{[\nu]} \) form a scalar product.

Separating diagonal and off-diagonal parts of \( \Lambda_1^{[\nu]} \) in (9) and (10) we obtain

\[
\chi^+_{J\downarrow} (q = 0, \omega) = \frac{1}{3N} \int \frac{dE}{2\pi} \text{tr} \left[ \sum_{m_n} I_1^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{im+}^{[\nu]} (E+\omega) \right. \]
\[
\times \Lambda_{1i}^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{ni+}^{[\nu]} (E+\omega),
\]

(11)

where

\[
\chi^+_{J\downarrow} (q = 0, \omega) = \frac{1}{3N} \int \frac{dE}{2\pi} \text{tr} \left[ \sum_{m_n} I_1^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{im+}^{[\nu]} (E+\omega) \right. \]
\[
\times \Lambda_{1i}^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{ni+}^{[\nu]} (E+\omega),
\]

(13)

Here only the locality of the irreducible particle-hole vertex \( I_1^{[\nu]} (E, E+\omega; \omega) \equiv I_1^{[\nu]} (E, E+\omega; E+\omega, E) \) 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 \( \nu = 1 \) can be solved without further assumptions on \( I_1^{[\nu]} \). Then by expanding \( \lambda_1^{[\nu]} \) and the effective spin-flip \( \Lambda_1^{[\nu]} \) in (6) and (7) to first order in \( \bar{q} \) and employing the cubic symmetry in the following one gets

\[
\chi^+_{J\downarrow} (q = 0, \omega) = \frac{1}{3N} \int \frac{dE}{2\pi} \text{tr} \left[ \sum_{m_n} I_1^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{im+}^{[\nu]} (E+\omega) \right. \]
\[
\times \Lambda_{1i}^{[\nu]} (E, E+\omega; \bar{q}) \sum_{m_n} G_{ni+}^{[\nu]} (E+\omega),
\]

(12)

where the notations \( \lambda_1^{[\nu]} = q \downarrow \bar{q} \uparrow, \quad \lambda_1^{[\nu]} = q \uparrow \bar{q} \uparrow \) have been introduced; under the trace \( \sum_{m_n} I_1^{[\nu]} \) and \( \Lambda_1^{[\nu]} \) form a scalar product.
Since the configurational averaging in (12) is beyond the CPA we make the factorization ansatz \( <\overline{A}|\psi>|_c = <A|\psi>_1 <\overline{\psi}|K\overline{\psi}>_C \) leading to

\[
\overline{K}_\sigma^\dagger(E_i + \omega, E_j) = <G^\dagger_\omega|E_i + \omega|G^\dagger_\omega\sigma>_{<\overline{\psi}|K\overline{\psi}>_C} = \frac{1}{N} \sum_{k} \overline{G}^\dagger_k (E_\omega) \overline{G}^\dagger_k \sigma (E) V_k \epsilon_k = 0 \tag{14}
\]

and \( \chi^+_\sigma (q = 0, \omega) = 0 \) due to time-reversal symmetry. \( \overline{G}^\dagger_k \sigma \) 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.,

\[
\chi^\dagger_\sigma (q = 0, \omega) = i \frac{1}{3N} \int \frac{d E}{2\pi} \sum_{k} \overline{G}^\dagger_k \sigma (E_\omega) \overline{G}^\dagger_k \sigma (E) V_k \epsilon_k = 0 \tag{15}
\]

Substituting (15) and

\[
\lim_{q \to 0} \frac{1}{q^2} \langle \overline{\psi}_+ | \psi^- | \rangle = \frac{1}{3N} \sum_{k} \langle \psi^- | \overline{\psi}_+ \rangle \overline{G}^\dagger_k \sigma (E_\omega) \overline{G}^\dagger_k \sigma (E) V_k \epsilon_k \tag{16}
\]

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

\[
D = \frac{1}{6\pi(n_n - n_n)} \int \frac{d E}{2\pi} \sum_{k} \left( \overline{G}^\dagger_k \sigma (E) - \overline{G}^\dagger_k \sigma (E) \right) \left( V_k \epsilon_k \right) \tag{17}
\]

where \( \mu \) 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, \( \overline{G}^\dagger_k \sigma \) is dressed in the CLA scheme \(^16^\). Then the correlation part expressed in terms of partially averaged causal functions reads

\[
\Sigma^\nu_{U\sigma} (z) = \int \frac{d E}{2\pi} G^\nu_{i\sigma} (\overline{E}) T^\nu_i (E + \overline{E}) , \quad (\nu = A, B) \tag{18}
\]

\[
T^\nu_i (E) = \left[ \frac{1}{U^\nu_i} + \int \frac{d E}{2\pi} G^\nu_{i\sigma} (\overline{E}) G^\nu_{i\sigma} (E - \overline{E}) \right]^{-1} \tag{19}
\]

where \( T^\nu_i \) is the effective two-particle vertex. The local Green function \( G^\nu_{i\sigma} (z) \) written as resolvent ( \( z \) being the complex energy) is renormalized by

\[
G^\nu_{i\sigma} (z) = \frac{F^\nu_{i\sigma} (z)}{1 - (\gamma^\nu_{i\sigma} (z) - \Sigma_{\sigma} (z)) F^\nu_{i\sigma} (z)} \tag{20}
\]

\[
\gamma^\nu_{i\sigma} (z) = \epsilon^\nu_{i\sigma} + \Sigma^\nu_{U\sigma} (z) \tag{21}
\]

\[
F^\nu_{i\sigma} (z) = \frac{1}{N} \sum_{k} \overline{G}^\dagger_k \sigma (z) \tag{22}
\]

\[
\Sigma_{\sigma} (z) = (z - \epsilon^\nu_{i\sigma} - \Sigma_{\sigma} (z))^{-1} \tag{23}
\]

\[
\Sigma^\nu_{U\sigma} (z) = c \epsilon^A_{\sigma} (z) + (1-c) \epsilon^B_{\sigma} (z) - [\epsilon^A_{\sigma} (z) - \epsilon^B_{\sigma} (z)] F^\nu_{i\sigma} (z) [\epsilon^B_{\sigma} (z) - \Sigma_{\sigma} (z)] \tag{24}
\]

\[
n = \sum_{\sigma} n_{\sigma} = - \frac{1}{\pi} \sum_{\sigma} \int \frac{d E}{2\pi} \text{Im} F^\nu_{i\sigma} (E) \tag{25}
\]

Here \( \Sigma_{\sigma} \) is the coherent potential, \( n \) is the average number of electrons per site. Contrary to the usual CPA \(^12^\), the atomic potential \( \gamma^\nu_{i\sigma} (z) \) ( \( i \) is dropped in (24)) becomes energy-dependent through the self-energy \( \Sigma^\nu_{U\sigma} (z) \) 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 \( \Sigma^\nu_{U\sigma} = U^\nu_i n_{i\sigma} \) , where \( n_{i\sigma}^\nu \) is the average electron number with spin \( \sigma \) at \( \nu \) sites given by

\[
n_{i\sigma}^\nu = - \frac{1}{\pi} \int \frac{d E}{2\pi} \text{Im} G^\nu_{i\sigma} (E) \tag{26}
\]
Taking into account the special vertex $I_\nu^i$ (E, $E + \omega; \omega$) =
$$= - T_{i \nu}^i (E + E + \omega) - T_{i \nu}^i (E + E + \omega),$$  the equations (7), (18)  and (19) with $\nu$ replaced by $\nu$ yield the identity \(^1\!^4\!)::

$$\omega \Lambda_{0i}^{[\nu]} (E, E + \omega; \omega) = e^{-i \mathbf{q} \cdot \mathbf{R}_i} G_{ij}^{[\nu]} (E + \omega) = - G_{ij}^{[\nu]} (E; \mathbf{e}^{-i \mathbf{q} \cdot \mathbf{R}_j}), \quad (27)$$

with

$$G_{ij}^{[\nu]} (E) = (E - \epsilon_i^\nu) \delta_{ij} - t_{ij} - \sum_{\nu} \Lambda_{0i}^{[\nu]} (E) \delta_{ij}, \quad (28)$$

where the site-diagonality of $\Lambda_{0i}^{[\nu]}$ has been used in (27). Hence, in the completely random version $\nu$, the local ladder approximation fulfills the Ward-Takahashi-type relation (27).

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

$$\hat{D} = D (n_+ - n_-) > 0$$  \quad (29)

may be found from the spectral representation

$$\chi^{+ - \nu} (\mathbf{q}, \omega) = - \frac{1}{2 \pi} \int_{0}^{\infty} d \omega \cdot \text{sign} \omega \cdot \frac{\epsilon_i}{\omega - \epsilon_i + i \epsilon} \hat{s}_i \cdot \hat{s}_j (\omega), \quad (30)$$

where the spectral density $\hat{s}_i \cdot \hat{s}_j (\omega) \geq 0$ is related to a configurationally averaged system. The magnon pole

$$\chi^{+ - \nu} (\mathbf{q}, \omega) = - \frac{n_+ - n_-}{\omega - D q^2 + i \epsilon}$$  \quad (31)

can be separated for small $q$ and $\omega$ (Goldstone theorem) from the Stoner continuum, since the individual excitations have vanishing spectral weight for $\mathbf{q} \to 0$. In (31) the damping is omitted, and the residue is written down only in the lowest order of $\epsilon$. The comparison of (30) and (31) leads to (29) \(^1\!^4\!).

In the present approximation the spin wave damping $\gamma_q$ entering into (31) instead of $\epsilon$ can be proved to be

$$\gamma_q = \frac{2}{N} \sum_{\mathbf{k}} \text{Im} \chi^{+ - \nu} (0, D \mathbf{q}^2) = \frac{-1}{3 \pi} \sum_{\mathbf{k}} \frac{D q^4}{(n_+ - n_- N) \mathbf{k}^+} \{ \text{Im} \chi^{+ \nu} (\mathbf{k}) \text{Im} \chi^{+ \nu} (\mathbf{k}) \}^2 (\mathbf{v}_m \cdot \mathbf{q})^2 \quad (32)$$

taking the same form as in RPA-CPA \(^3\!^8\!^8\); 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 \(^2\!^2\) 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:

$$\rho_0 (E) = \frac{1}{N} \sum_{\mathbf{k}} \delta (E - \epsilon_i^\nu (\mathbf{q})) = \frac{2}{\pi w} \left[ 1 - \left( \frac{E}{w} \right)^2 \right]^{\frac{1}{2}} \theta (w - |E|), \quad (33)$$

$$\frac{1}{N} \sum_{\mathbf{k}} \delta (E - \epsilon_i^\nu (\mathbf{q})) (\mathbf{v}_m \cdot \mathbf{k})^2 = \frac{2 v_m^2}{\pi w} \left[ 1 - \left( \frac{E}{w} \right)^2 \right]^{\frac{3}{2}} \theta (w - |E|), \quad (34)$$

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

$$F_\sigma (z) = \frac{2}{w} \left( \frac{z}{w} - i \sqrt{1 - \frac{z^2}{w^2}} \right), \quad \frac{z}{w} = \frac{z - \Sigma_\sigma (z)}{w}. \quad (35)$$
To make (35) univalent we take that branch in the \( z_0 \)-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

\[
D = \frac{1}{6\pi(n_+ - n_-)} \text{Im} \int d\varepsilon [\Pi_{\sigma\sigma}^{rr}(E,E) + \Pi_{\sigma+\sigma}^{rr}(E,E) - 2 \Pi_{\sigma+\sigma}^{rr}(E,E)]
\]

(36)

with the abbreviations

\[
\Pi_{\sigma\sigma}^{rr}(E,E) = \Pi_{\sigma\sigma}^{rr}(E^+,E^+), E^+ = E + i0,
\]

and

\[
\Pi_{\sigma+\sigma}^{rr}(z,z') = \frac{1}{N} \sum_{\kappa} \sum_{\kappa'} \sigma \sigma' \Pi_{\sigma\sigma}(z) \Pi_{\sigma\sigma}(z')(V_{\kappa} - \epsilon_{\kappa})^2
\]

(37)

we find in performing the \( \kappa \)-sum with (34) by the residue method the current polarization parts

\[
\Pi_{\sigma\sigma}^{rr} = \frac{2\sqrt{2}}{3w^2} (3z^2 - \frac{3}{2} - 3iz\sqrt{1 - z^2}),
\]

\[
z_\sigma = \frac{E^+ - \Sigma_{\sigma}(E^+)}{w},
\]

(38)

\[
\Pi_{\sigma+\sigma}^{rr} = \frac{2\sqrt{2}}{3w^2} (z^2 + \frac{3}{2} + 3iz\sqrt{1 - z^2}).
\]

(39)

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

\[
D = \frac{2\sqrt{2}}{3\pi w} \text{Im} \int d\varepsilon [(z_+ - z_-)^2 - i\sqrt{1 - z_+^2}(3z_+ - \frac{2(1 - \sqrt{1 - z_+^2})}{z_+ - z_-}) - i\sqrt{1 - z_-^2}(3z_- - \frac{2(1 - \sqrt{1 - z_-^2})}{z_+ - z_-})],
\]

(40)

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

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

\[
\sigma = \frac{2}{6\pi} N \sum_{\alpha} \left[ \Pi_{\sigma\sigma}^{rr}(\mu,\mu) - \text{Re} \Pi_{\sigma\sigma}^{rr}(\mu,\mu) \right] \sigma_{\sigma\sigma}
\]

(41)

including Green functions renormalized by electron correlations within the CLA. Here \( \Pi_{\sigma\sigma}^{rr}(\mu,\mu) = \Pi_{\sigma\sigma}^{rr}(\mu^+,\mu^-) \), \( \mu^- = \mu - 10 \), \( V \) is the volume of the system, and \( e \) is the unit charge. By inserting (38) and (39) with the replacement \( \Pi_{\sigma\sigma}^{rr} = \Pi_{\sigma\sigma}^{rr} \left[ z_+ \rightarrow z_\sigma, z_\sigma \rightarrow z_\sigma^+ \right] \) into (41) we get the spin-dependent dc conductivity (for \( \text{Im} \Sigma_{\sigma}(\mu^+) < 0 \))

\[
\sigma_{\sigma} = \frac{\mu^+ - \Sigma_{\sigma}(\mu^+)}{w} = \frac{e^2 v_m N}{3\pi v_m N}.
\]

(42)

The numerical analysis is performed as follows:

Choose the parameters \( w, e, U = 2 \), \( U_A, U_B, U \) fixed, \( n \); 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 \( \varepsilon \)-integration.

\[ Figure \ 1 \] shows the transition region between weak and strong ferromagnetism versus the strengths of the intra-atomic Coulomb repulsion \( U \) 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 [23/124], but not in the context of spin waves. The RPA-CPA results (a) for the stiffness constant \( D \) (in units of \( d_0^{-2} \)) refer to the instability of the ferromagnetic ground state against spin wave excitations. Note that a crossing of the spin-dependent dc conductivities \( \sigma_{\sigma}(\mu) \) is found (cf. [24]). The component and average magnetizations \( m' = n' - n' \) and \( m = n - n' \), resp., are drawn in Fig. 1d.

\[ Figure \ 2 \] represents a confined region of stable (mainly saturated) ferromagnetism \( (D > 0 \) (b), \( m' > 0 \) (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 a change of the spin arrangement. Note that the maxima of \( D \) and \( \sigma \), (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 that our model calculation can be justified only for small Fe concentrations. Note that for pure Ni the stiffness constant is found close to \( D_{Ni} = 555 \text{ meV A}^2 \) measured at 4.2 \( K \)\(^{11}\).

Electron correlation effects on the stiffness constant \( D \) in NiPd alloys are studied in Fig. 4, and a comparison with \(^{125}\) 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 \( n = c n_{Pd} + (1 - c) n_{Ni} \), 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 \( U^{\nu} \) are dressed self-consistently yielding the two-particle vertices \( T_i(E + \epsilon) \),
Fig. 3. Spin wave stiffness constant $D$ versus $c$ for $\text{Fe}_c\text{Ni}_{1-c}$ alloys. $D$ values ($x$) based on the coherent ladder approximation with $(a, b, c, d, u, v, n) = (0.5, -0.24, 0, 2.66, 3.4, 0.6)$ ($2w = 4.15$ eV, $a = 4\text{Å}$ in absolute units in b)). Comparison with a) results computed in $^7(1), ^8(2), ^9(3), ^{10}(4)$ and a), b) experimental data given in $^7(1), ^8(2$), $^9(3), ^{10}(4$) and a).

especially $\Gamma^\nu = T^\nu(2_\mu)$ 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-wave-length limit $\omega_q = D q^2$. Although a single-band Hubbard model with simplified band structure and diagonal dis-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.

Fig. 4. $\text{Pd}_c\text{Ni}_{1-c}$ alloys treated by using the coherent ladder approximation with the set $(2w)^{1/2}_\text{Pd}, (2w)^{1/2}_\text{Ni}$, $(c^{1/2}_\text{Pd}, c^{1/2}_\text{Ni}, n^{1/2}_\text{Pd}, n^{1/2}_\text{Ni}) = (6.05$ 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 $^7(1), ^8(2,3,4$) and a), b) $D$ in absolute units $(a = 3.8 \text{Å})$, c) partial magnetizations $m^\nu$, and d) effective Coulomb interactions $\Gamma^\nu$ and $\Gamma^\nu$ versus $c$.
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