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Влияние межэлектронных корреляций на коэффициент жесткости спиновых волн в ферромагнитных металлах

Использование микроскопической теории ферми- жидкости позволяет рассчитывать энергию длинноволновых спиновых возбуждений в ферромагнитных переходных металлах при нулевой температуре. Коэффициент жесткости D включает электрон-электронные корреляции, учитываемые в рамках модели Хаббарда в горизонтальном лестничном приближении. Численные результаты для D получены на основе самосогласованной перенормировки спинового расщепления зоны. Проведено сравнение с результатами рассеяния нейтронов для никеля.

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Electron Correlation Effects on the Spin Wave Stiffness Constant in Itinerant Ferromagnets

A microscopic Fermi liquid approach is chosen to calculate the energy of long-wavelength spin waves in ferromagnetic transition metals at zero temperature. The stiffness constant D involves electron-electron correlations treated within the horizontal ladder approximation for the bare Hubbard interaction. Numerical results for D are obtained by performing self-consistently an energy-dependent renormalization of the band splitting. A comparison with neutron scattering data for nickel is given.

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

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The stability of ferromagnetism in metals is connected with the existence of long-wavelength spin waves below the Stoner gap in the particle-hole excitation spectrum. The spin wave energy $\omega_q = Dq^2$ for cubic crystals is determined by a pole of the transverse susceptibility $\chi^{+-}(\vec{q},\omega)$ yielding the spin wave stiffness constant

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

where $2\langle S^z\rangle$ is the magnetization per lattice site. An alternative formula

$$D = \frac{1}{2\langle S^z\rangle}\left[\lim_{q\to 0}\frac{1}{q^2}\langle[S^+_{\vec{q}}, qJ^-_{-\vec{q}}]\rangle - \lim_{\omega\to 0}\lim_{q\to 0}\chi_J^{+-}(\vec{q},\omega)\right] \qquad (2)$$

was derived in terms of the spin current-spin current response $\chi_J^{+-}(\vec{q},\omega)$ by Edwards and Fisher /1/. To describe the itinerant d-electrons in ferromagnetic transition metals we choose the spin-rotational invariant Hubbard Hamiltonian /2/

$$H = \sum_{\vec{k}\sigma}\epsilon_{\vec{k}} n_{\vec{k}\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (3)$$

where $n_{\vec{k}\sigma}$ $(n_{i\sigma})$ is the occupation number operator for Bloch (Wannier) states with spin σ, $\epsilon_{\vec{k}}$ is the band energy, and U denotes the bare local interaction. For this model the transverse spin density and current operators are given by $S^+_{\vec{q}} = \frac{1}{\sqrt{N}}\sum_{\vec{k}} c^+_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}$ (or $S^-_{-\vec{q}} = (S^+_{\vec{q}})^+$) and $qJ^+_{\vec{q}} = \frac{1}{\sqrt{N}}\sum_{\vec{k}}(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}})c^+_{\vec{k}\uparrow}c_{\vec{k}+\vec{q}\downarrow}$ (or $J^-_{-\vec{q}} = (J^+_{\vec{q}})^+$), resp., where $c^+_{\vec{k}\sigma}$ creates an electron in the state $|\vec{k}\sigma\rangle$, N is the number of lattice sites.

The aim of this paper is to renormalize the stiffness constant D by electron correlations using the local ladder approximation (LLA) [3] in the particle-particle channel. Within a microscopic Fermi liquid approach (cf. [4]) at zero temperature the susceptibilities in (1) and (2) can be expressed in terms of causal Green functions as follows

$$\chi^{+-}(\vec{q},\omega) = -\langle\langle S^{+}_{\vec{q}}, S^{-}_{-\vec{q}}\rangle\rangle_{\omega} =$$

$$= \frac{i}{N}\int \frac{dE}{2\pi}\sum_{\vec{k}} G_{\vec{k}+\vec{q}\downarrow}(E+\omega)\Lambda_{0\vec{q}\downarrow\uparrow}(E+\omega,E)\,G_{\vec{k}\uparrow}(E)\,, \tag{4}$$

$$\Lambda_{0\vec{q}\downarrow\uparrow}(E+\omega,E) = 1 - \int \frac{d\bar{E}}{2\pi}\, i I_{\downarrow\uparrow\uparrow\downarrow}(E+\omega,\bar{E};-\omega)\times$$

$$\times \frac{1}{N}\sum_{\vec{k}} G_{\vec{k}+\vec{q}\downarrow}(\bar{E}+\omega)\Lambda_{0\vec{q}\downarrow\uparrow}(\bar{E}+\omega,\bar{E})\,G_{\vec{k}\uparrow}(\bar{E})\,, \tag{5}$$

$$q^2\chi_J^{+-}(\vec{q},\omega) = -\langle\langle qJ^{+}_{\vec{q}}, qJ^{-}_{-\vec{q}}\rangle\rangle_{\omega} =$$

$$= \frac{i}{N}\int \frac{dE}{2\pi}\sum_{\vec{k}} (\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}})\,G_{\vec{k}+\vec{q}\downarrow}(E+\omega)\Lambda_{1\underset{\downarrow}{\vec{k}}+\vec{q}\underset{\uparrow}{\vec{k}}}(E+\omega,E)\,G_{\vec{k}\uparrow}(E)\,, \tag{6}$$

$$\Lambda_{1\underset{\downarrow}{\vec{k}}+\vec{q}\underset{\uparrow}{\vec{k}}}(E+\omega,E) = \epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}} - \int \frac{d\bar{E}}{2\pi}\, i I_{\downarrow\uparrow\uparrow\downarrow}(E+\omega,\bar{E};-\omega)\times$$

$$\times \frac{1}{N}\sum_{\vec{k}'} G_{\vec{k}'+\vec{q}\downarrow}(\bar{E}+\omega)\Lambda_{1\underset{\downarrow}{\vec{k}'}+\vec{q}\underset{\uparrow}{\vec{k}'}}(\bar{E}+\omega,\bar{E})\,G_{\vec{k}'\uparrow}(\bar{E})\,. \tag{7}$$

Here only the locality of the irreducible particle-hole vertex $I_{\downarrow\uparrow\uparrow\downarrow}$ has been assumed. Hence the prescription (2) instead of (1) is favoured, because the Bethe-Salpeter-type equation (7) can be solved without further assumptions. By employing time-reversal symmetry the effective spin-flip current Λ_1 can be found at first order of $\vec{q}$ immediately from (7), giving rise to vanishing vertex corrections in (6), i.e.,

$$\chi_J^{+-}(\vec{q}=0,\omega) = \frac{i}{3N}\int \frac{dE}{2\pi}\sum_{\vec{k}} G_{\vec{k}\downarrow}(E+\omega)\,G_{\vec{k}\uparrow}(E)\,(\nabla_{\vec{k}}\epsilon_{\vec{k}})^2\,. \tag{8}$$

Inserting (8) and $\lim_{q\to 0}\frac{1}{q^2}\langle[S^{+}_{\vec{q}}, qJ^{-}_{-\vec{q}}]\rangle = \frac{1}{6N}\sum_{\vec{k}\sigma}\langle n_{\vec{k}\sigma}\rangle\nabla^2_{\vec{k}}\epsilon_{\vec{k}}$ into (2) and going over to retarded ("r") Green functions we obtain

$$D = \frac{1}{6\pi(n_\uparrow - n_\downarrow)}\,\mathrm{Im}\int_{-\infty}^{\mu} dE\,\frac{1}{N}\sum_{\vec{k}}\left(G^{r}_{\vec{k}\uparrow}(E) - G^{r}_{\vec{k}\downarrow}(E)\right)^2(\nabla_{\vec{k}}\epsilon_{\vec{k}})^2\,, \tag{9}$$

where n_σ is the average number of σ electrons per site, and μ denotes the Fermi level. This expression for D reduces to the usual RPA result (cf., e.g., [5]), provided that the one-particle propagator $G_{\vec{k}\sigma}$ is taken in the Hartree-Fock approximation. In the present calculation, however, $G_{\vec{k}\sigma}$ is dressed in the LLA-scheme [3]

$$\Sigma_\sigma(E) = \int \frac{d\bar{E}}{2\pi i}\,G_{-\sigma}(\bar{E})\,T(E+\bar{E})\,,\quad T(E) = \left[\frac{1}{U} + \int \frac{d\bar{E}}{2\pi i}\,G_\sigma(\bar{E})\,G_{-\sigma}(E-\bar{E})\right]^{-1}, \tag{10}$$

$$n = \sum_\sigma n_\sigma = \sum_\sigma \int \frac{dE}{2\pi i}\,G_\sigma(E)\,,\qquad G_\sigma(E) = \frac{1}{N}\sum_{\vec{k}} G_{\vec{k}\sigma}(E)\,, \tag{11}$$

$$G^{-1}_{\vec{k}\sigma}(E) = E - \epsilon_{\vec{k}} - \Sigma_\sigma(E)\,. \tag{12}$$

Taking into account the special vertex $I_{\downarrow\uparrow\uparrow\downarrow}(E+\omega,\bar{E};-\omega) = -T_{\uparrow\downarrow\uparrow\downarrow}(E+\bar{E}+\omega) = -T(E+\bar{E}+\omega)$, (5),(7), (10) and (12) yield the identity

$$\omega\Lambda_{0\vec{q}\downarrow\uparrow}(E+\omega,E) + \Lambda_{1\underset{\downarrow}{\vec{k}}+\vec{q}\underset{\uparrow}{\vec{k}}}(E+\omega,E) = G^{-1}_{\vec{k}+\vec{q}\downarrow}(E+\omega) - G^{-1}_{\vec{k}\uparrow}(E)\,. \tag{13}$$

Thus the LLA satisfies the Ward-Takahashi relation (13).

The condition $\hat{D} = D(n_\uparrow - n_\downarrow) > 0$ following from the spectral representation of $\chi^{+-}(\vec{q},\omega)$ ensures the stability of the ferromagnetic ground state. Here the spin wave damping $\gamma_q = \frac{q^2}{n_\uparrow - n_\downarrow} \mathrm{Im}\chi_J^{+-r}(0, Dq^2)$ can be proved to be small at least of order q^4.

The numerical calculation is performed as follows: Choose the parameters U and the electron concentration n, a semielliptic unperturbed density of states (bandwidth 2w, in reduced units 2w = 1) and solve the self-consistency loop (10) to (12); carry out the $\vec{k}$-summation in (9) by assuming $\frac{1}{N}\sum_{\vec{k}} \delta(E-\epsilon_{\vec{k}})(\nabla_{\vec{k}}\epsilon_{\vec{k}})^2 = \frac{2v_m^2}{\pi w}(1-(\frac{E}{w})^2)^{3/2}\theta(w-|E|)$ (v_m is or order wa, a is the lattice spacing); and use these results to get D from (9) via E-integration.

Fig. 1a shows the spin wave stiffness constant D in units of $d_0 = \frac{2}{9}wa^2$ in the stable ferromagnetic case ($D > 0$, $n_\uparrow > n_\downarrow$). For comparison Hartree-Fock results are given which qualitatively correspond to /5/. The stable ferromagnetic solutions in LLA confine the region obtained from the zeroes of the inverse paramagnetic susceptibility /6/. Contrary to a constant effective interaction of the Kanamori type (cf., e.g., /7/) the renormalization of U here is given by T(E+E), especially $\Gamma = T(2\mu)$ is plotted in *Fig. 1b*. According to the adequacy of the LLA, Γ is strongly diminished for small n. The *Table* lists numerical results of D obtained for 2w and bare U values related to nickel /7/ with 0.6 holes per atom in the d band. It turns out that within the predicted parameter range D values are found close to the inelastic neutron scattering data for Ni, compare, e.g., $D_{Ni} = 555\ meV\AA^2$ at 4.2*K* due to Mook et al. /8/. *Fig. 2a* exhibits that D_{Ni} fits into the stable (here saturated) ferromagnetic region of the model calculation, where the effective interaction at the renormalization point 2μ is cast in the range 4-8 *eV* (*Fig. 2b*) typifying d metals.

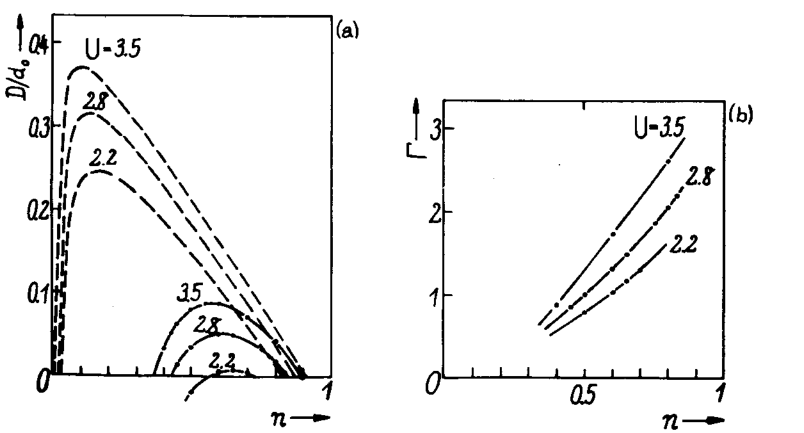

Fig. 1. a) Spin wave stiffness constant D(•) *compared with Hartree-Fock results* (---) *and b) effective two-particle vertex* Γ *vs.* n *for different values of* U *in units of the bandwidth* 2w.

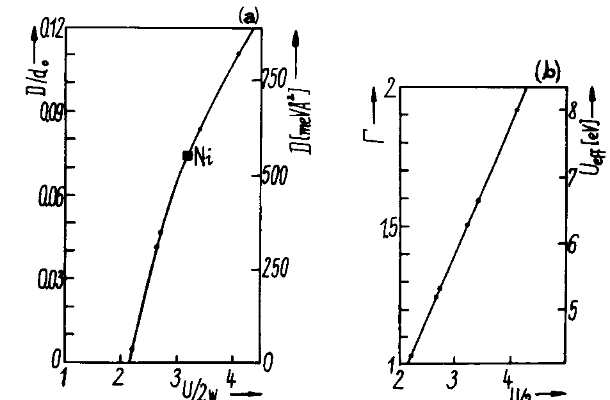

Fig. 2. a) Spin wave stiffness constant D *and b) effective two-particle vertex* Γ *vs.* U/2w *for* n=0.6. *The scales refer to reduced units* ($D/d_0, \Gamma$) *and to absolute units* ($D, U_{eff} = 2w\Gamma$) *with* 2w = *4.15 eV,* a = 4 Å.

To summarize: taking into account electron-electron correlations in itinerant ferromagnets we have found reasonable values of D, although a single-band Hubbard model with simplified band structure was used.

Table

Variation of D with U and a at fixed n = 0.6, 2w = 4.15 *eV*

U [eV]	D/d_0	D [meVÅ²] a = 3.52 Å	D [meVÅ²] a = 3.8 Å	D [meVÅ²] a = 4 Å	D [meVÅ²] a = 4.25 Å
11.27	0.0471	269	314	348	392
13.28	0.0749	428	499	553	624
14.11	0.0838	479	558	618	698
16.99	0.1111	635	740	820	925

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