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Перенормировка спинволновой жесткости в сплавах на никелевой основе

Исследуется спинволновой спектр $\omega_q = Dq^2$ металлических сплавов A_cB_{1-c} с учетом недиагонального беспорядка и локальных электрон-электронных корреляций. Коэффициент D, содержащий вершинные поправки, определяемые случайными интегралами переноса в аддитивном пределе, рассчитан в рамках когерентного лестничного приближения. Представлены численные результаты по D в сплавах NiPd и NiPt для всех концентраций c. Расчеты D отражают наблюдаемые критические концентрации для магнитного фазового перехода и могут служить критерием стабильности ферромагнитного основного состояния.

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Renormalization of the Spin Wave Stiffness in Ni -Based Alloys

The spin wave spectrum $\omega_q = Dq^2$ of metallic A_cB_{1-c} alloys is investigated by taking into account off-diagonal disorder and local electron-electron correlations. The stiffness coefficient D involving vertex corrections due to additively random transfer integrals is calculated within the coherent ladder approximation. Numerical results of D are presented for NiPd and NiPt alloys in the whole range of the concentration c. The computed D values confirm the observed critical concentrations for the magnetic phase transition and testify to the stability or instability of the ferromagnetic ground state.

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

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Some transition metal alloys exhibit magnetic critical concentrations[1,2,3]. This paper deals with the stability of the ferromagnetic state in NiPd and NiPt alloys against long-wavelength spin waves of the energy $\omega_q = Dq^2$. Including off-diagonal disorder of the additive type the spin wave stiffness constant D for A_cB_{1-c} alloys at zero temperature was derived in[4] on the basis of a single-band random Hubbard model, so that

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

where

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

$$\mathcal{G}_{\vec{k}\sigma}(z) = (z - \epsilon^B - t^{BB} s(\vec{k}) - \Sigma_\sigma(\vec{k},z))^{-1}, \quad (3)$$

$$\Sigma_\sigma(\vec{k},z) = \sigma_{0\sigma}(z) + 2\sigma_{1\sigma}(z) s(\vec{k}) + \sigma_{2\sigma}(z) s^2(\vec{k}), \quad (4)$$

$$n = \sum_\sigma n_\sigma = -\frac{1}{\pi N} \sum_{\vec{k}\sigma} \int_{-\infty}^{\mu} dE \, \mathrm{Im} \, \mathcal{G}_{\vec{k}\sigma}(E^+). \quad (5)$$

Here μ denotes the Fermi energy, n is the average number of electrons per site, N is the number of lattice sites, $E^+ = E + i0$, and $s(\vec{k}) = \sum'_{j(\neq i)} e^{i\vec{k}(\vec{R}_i - \vec{R}_j)}$. The nearest-neighbour hopping integrals $t^{\nu\mu}$ are related by $t^{AB} = \frac{1}{2}(t^{AA} + t^{BB})$. The coherent self-energy parts $\sigma_{0\sigma}$, $\sigma_{1\sigma}$, $\sigma_{2\sigma}$ will be determined from the off-diagonal CPA conditions [4]. Electron-electron correlations are taken into account by

$$\left.\begin{aligned} \Sigma^{\nu}_{Uii\sigma}(E) &= \int \frac{dE'}{2\pi i} G^{\nu}_{ii-\sigma}(E')\Gamma^{\nu}_{i}(E+E'), \qquad (\nu = A,B) \\ \Gamma^{\nu}_{i}(E) &= [\frac{1}{U^{\nu}_{i}} + \int \frac{dE'}{2\pi i} G^{\nu}_{ii\sigma}(E')G^{\nu}_{ii-\sigma}(E-E')]^{-1}, \end{aligned}\right\} \tag{6}$$

where U^{ν}_{i} and Γ^{ν}_{i} represent the bare and effective intra-atomic Coulomb interactions, resp., and the partially averaged causal Green function $G^{\nu}_{ii\sigma}(E)$ is given in [4]. The self-energy $\Sigma^{\nu}_{Uii\sigma}$ renormalizes the atomic potential as $\tilde{\epsilon}^{\nu}_{i\sigma}(z) = \delta^{\nu}_{i} + \Sigma^{\nu}_{Uii\sigma}(z)$, where $\delta^{A}_{i} = \epsilon^{A} - \epsilon^{B}$ and $\delta^{B}_{i} = 0$.

The numerical study of D within the present coherent ladder approximation (CLA) is still outstanding. To perform the $\vec{k}$-summation in (2) we choose a simplified mean-square velocity

$$\frac{1}{N}\sum_{\vec{k}} \delta(E - \epsilon^{B}_{\vec{k}})(\nabla_{\vec{k}}\epsilon^{B}_{\vec{k}})^2 = \frac{2(v^{B}_{m})^2}{\pi w^{B}}(1-(\frac{E}{w^{B}})^2)^{3/2}\theta(w^{B}-|E|), \tag{7}$$

where $\epsilon^{B}_{\vec{k}} = t^{BB}s(\vec{k})$, $\epsilon^{B} = 0$, w^{B} (here $w^{B} = 6t^{BB}$) is the half-bandwidth of the unperturbed B-band, and v^{B}_{m} is of order $w^{B}a$ (a : lattice spacing). By inserting (7) into (2) combined with (3) and (4) we get

$$\begin{aligned} \Pi_{\sigma\sigma'}(E^+,E^+) = \frac{2(v^{B}_{m})^2}{\pi}\{&[1 + \frac{12}{w^{B}}(\sigma_{1\sigma}(E^+) + \sigma_{1\sigma'}(E^+)) + \\ &+ \frac{36}{(w^{B})^2}(\sigma_{1\sigma}(E^+) + \sigma_{1\sigma'}(E^+))^2]H_{0\sigma\sigma'}(E^+,E^+) + \\ &+ \frac{72}{w^{B}}(\sigma_{2\sigma}(E^+) + \sigma_{2\sigma'}(E^+))[1 + \frac{6}{w^{B}}(\sigma_{1\sigma}(E^+) + \\ &+ \sigma_{1\sigma'}(E^+))]H_{1\sigma\sigma'}(E^+,E^+) + \end{aligned} \tag{8}$$

$$\begin{aligned} &+ [\frac{36}{w^{B}}(\sigma_{2\sigma}(E^+) + \sigma_{2\sigma'}(E^+))]^2 H_{2\sigma\sigma'}(E^+,E^+) + \\ &+ \frac{36}{(w^{B})^2}[\sigma_{2\sigma}(E^+)\hat{F}_{\sigma'}(E^+) + \sigma_{2\sigma'}(E^+)\hat{F}_{\sigma'}(E^+)]\}, \end{aligned}$$

where

$$H_{\ell\sigma\sigma'}(z,z') = \int_{-1}^{1} d\xi\,(1-\xi^2)^{3/2}\xi^{\ell}\mathcal{G}_{\sigma}(z;\xi)\mathcal{G}_{\sigma'}(z';\xi), \tag{9}$$

$(\ell = 0,1,2)$

$$\hat{F}_{\sigma}(z) = \int_{-1}^{1} d\xi\,(1-\xi^2)^{3/2}\mathcal{G}_{\sigma}(z;\xi), \tag{10}$$

$$\mathcal{G}_{\sigma}(z;\xi) = [z - \sigma_{0\sigma}(z) - (w^{B} + 12\sigma_{1\sigma}(z))\xi - 36\,\sigma_{2\sigma}(z)\xi^2]^{-1} \tag{11}$$

The integrals (9) and (10) can be calculated analytically by the residue method (cf. [5]). Analogously, the $\vec{k}$-sum in (5) involving the averaged propagator $\mathcal{G}_{\vec{k}\sigma}$ is obtained by assuming a semi-elliptic density of states for the unperturbed B-band (bandwidth $2w^{B}$).

The numerical analysis is carried out as follows. Choose the parameters w^{A}, w^{B} (in reduced units $w^{B} = 1/2$), ϵ^{A}, U^{A}, U^{B}, c, and $n = cn^{A} + (1-c)n^{B}$; solve the self-consistency problem (3) to (6) completed by the explicit form of $G^{\nu}_{ii\sigma}$ and the CPA requirements $\langle \tau^{\nu}_{\ell\sigma} \rangle_{c} = 0$ $(\ell = 0,1,2)$ given in [4]; and substitute the resultant $\sigma_{\ell\sigma}$ in (8) to get D from (1). For NiPd and NiPt alloys we adopt the pure values (cf. [6]) (U^{Ni}, U^{Pd}, U^{Pt}, $2w^{Ni}$, $2w^{Pd}$, $2w^{Pt}$) = (14.11, 9.17, 6.61, 4.15, 6.05, 7.8) *eV*, and $n^{Ni} = 0.6$, $n^{Pd} = n^{Pt} = 0.4$ corresponding to the number of d-holes per atom. Moreover, we use $\epsilon^{Ni} - \epsilon^{Pd} = 0$ and $\epsilon^{Ni} - \epsilon^{Pt} = 0$.

Fig. 1 shows CLA results of the stiffness coefficient D in units of $d_0 = \frac{2}{9}w^{B}a^2$ for Pd_cNi_{1-c} ($w^{B} = w^{Ni}$) and Ni_cPd_{1-c} ($w^{B} = w^{Pd}$) alloys and D/D_{Ni} compared with experimental data [7]. For pure Ni we get at $a = 3.8$ Å $D_{Ni} = 558$ *meVÅ*^{2} close to the observed value [8]. The peak of D near the critical concentration $c_{cr} = 2.3$ at. % Ni in Pd [1,3] refers to considerable spin fluctuations ($D/d_0 = -0.81$ at $c = 0.025$) at the paramagnetic-ferromag-

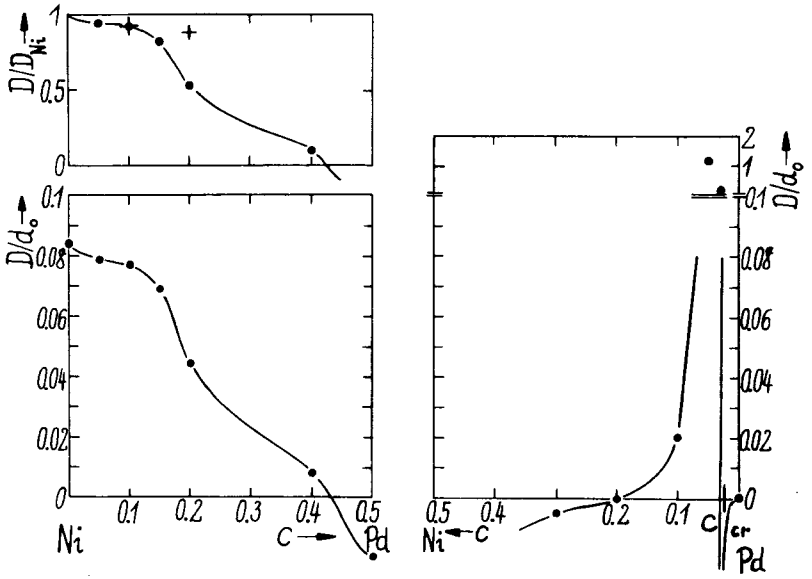

Fig. 1. Variation of the spin wave stiffness D(•) *with composition of* NiPd *alloys. Crosses* (+) *denote experimental values* [7].

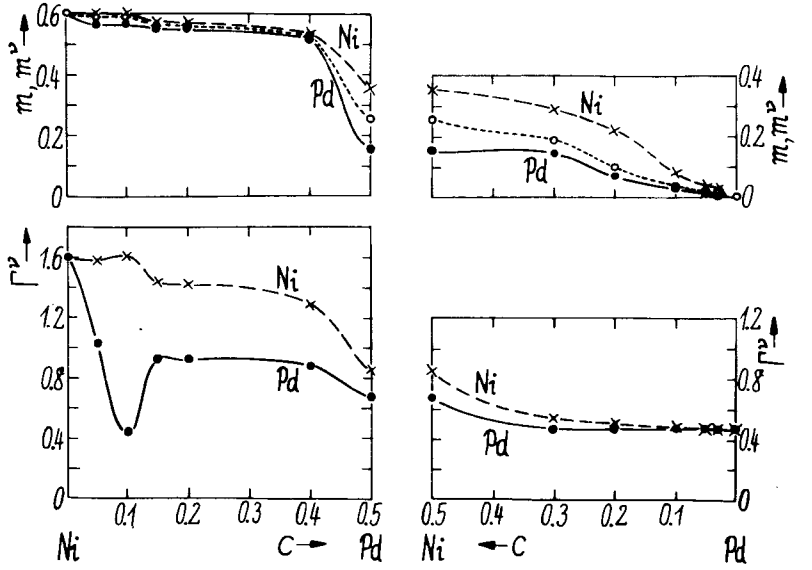

Fig. 2. Totally averaged magnetization m(o), *partially averaged* (× – Ni, • – Pd) *magnetizations* m^ν *and effective Coulomb interactions* Γ^ν *vs. concentration* c *of* NiPd *alloys.*

netic phase transition. Susceptibility measurements [1] near c_{cr} reflect such a bulk ferromagnetism (cf. the concept of giant moments). An unstable region $D < 0$ is found at intermediate c. For the alloy of *Fig. 1* the average magnetization $m = n_\uparrow - n_\downarrow$, the partial magnetizations $m^\nu = n_\uparrow^\nu - n_\downarrow^\nu$ with $n_\sigma^\nu = -\frac{1}{\pi}\int_{-\infty}^{\mu} dE\, \mathrm{Im}\, G_{ii\sigma}^\nu(E^+)$, and the special reduced value $\Gamma^\nu = \Gamma_1^\nu(2\mu)$ of the vertex function $\Gamma_1^\nu(E, E')$ are plotted in *Fig. 2*. The absolute values of Γ^ν vary between about 6.5 *eV* (Ni -rich) and 3 *eV* in the Pd -rich region, wherein m increases with c (cf. [1]). *Figure 3* represents the numerical results of m , m^ν (a) and D (b) for Pt_cNi_{1-c}

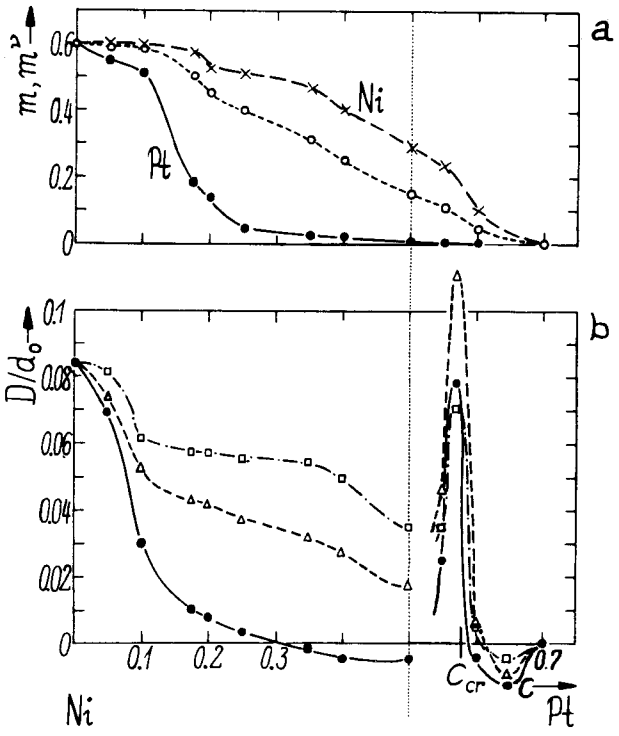

Fig. 3. a) Total and partial magnetizations m(o), m^ν (× – Ni, • – Pt), *b) spin wave stiffness* D *with* (•) *and without* (Δ, □) *vertex corrections vs. concentration* c *of* NiPt *alloys.*

and $Ni_c Pt_{1-c}$ alloys (divided by a vertical dashed line). The onset of ferromagnetism near $c_{cr} \approx 42$ at.% Ni in Pt is also accompanied by a peak in D. Note that c_{cr} is confirmed by susceptibility and magnetization measurements [2]. The values of $D(\bullet)$ in *Fig. 1* and *Fig. 3* involve vertex corrections proportional to $\sigma_{1\sigma}$ and $\sigma_{2\sigma}$ in (2). Such terms arise from the randomness of the current $\vec{j}^{\{\nu\}} = \vec{j}^{(0)} + \vec{j}^{(1)\{\nu\}}$ [4] ($\vec{j}^{(0)}$: nonrandom part). Without vertex corrections, $D[\vec{j}^{(0)}](\Delta)$ and $D[\vec{j}^{(0)} + \langle \vec{j}^{(1)\{\nu\}} \rangle_c](\square)$ overestimate the stable behaviour in *Fig. 3b*.

The self-consistent CLA renormalization of D, which supposes bare model parameters and simple input functions as (7), provides a distinct check on stable ferromagnetism in NiPd and NiPt alloys, especially for the dynamics near c_{cr}.

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