ОБЪЕДИНЕННЫЙ
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ДУБНА

261/11-79
E17 - 11960

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Submitted to "physica status solidi"

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E17 - 11960

Спинволновая жесткость в узкозонных ферромагнитных сплавах со случайными интегралами перескока

Получена спинволновая жесткость D в ферромагнитных бинарных металлических сплавах при нулевой температуре на основе хаотической модели Хаббарда с учетом диагонального и недиагонального беспорялков. Мы ограничились флуктуациями интегралов перескока в аддитивном пределе. С помощью обобщенной версии CPA вычислены вершинные поправки к D за счет случайности поперечного спинового тока. Коэффициент D перенормируется в рамках когерентного горизонтального лестничного приближения, включающего электрон-электронные корреляции. Обсуждаются устойчивость и затухание спиновых волн, тождества Уорда и электропроводность.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1978

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E17 - 11960

Spin Wave Stiffness Constant of Narrow-Band Ferromagnetic Alloys with Random Hopping

The spin wave stiffness constant D of ferromagnetic binary metallic alloys is derived at zero temperature from a random Hubbard model including diagonal and off-diagonal disorder. The fluctuations of the hopping integrals are restricted to the additive limit. Vertex corrections to D due to the randomness of the transverse spin current are calculated in an extended CPA. D is renormalized by electron-electron correlations within the coherent horizontal ladder approximation. Stability and damping of the spin waves, Ward relations, and the electrical conductivity are discussed.

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

Preprint of the Joint Institute for Nuclear Research. Dubna 1978

1. INTRODUCTION

Spin wave excitations in ferromagnetic transition metal alloys are characterized by the stiffness constant D which is affected by both electron-electron correlations and disorder. The itinerant d-electrons responsible for ferromagnetism can be described by a random Hubbard model[1] having spin rotational symmetry. Thus in the long-wavelength region one can extract in principle, according, e.g., to Bogolubov's $1/q^2$ -theorem from the broken symmetry (cf.[2]), a gapless magnon branch $\omega_q = Dq^2$ below the Stoner gap in the particle-hole excitation spectrum.

Previous studies of D in random itinerant-electron ferromagnets are mostly based[3 to 7] on the random phase approximation (RPA) combined with the coherent potential approximation (CPA)[8], where the electron-electron interaction is taken into account in the Hartree-Fock approximation and only diagonal disorder is included. In general, the hopping integrals in real disordered alloys are random. Hence, owing to the relationship between D and the transverse spin current susceptibility[9], there may

appear vertex corrections arising from the random current operator. In the RPA decoupling scheme[10] these vertex corrections have not been considered.

In this paper we choose a microscopic Fermi liquid approach (cf.[11]) at zero temperature to derive D for narrow-band alloys involving random transfer energies in the additive limit. In Section 2 the vertex corrections due to the random current are calculated in generalizing the diagonal disorder treatment[11]. The stiffness constant D is renormalized within the coherent ladder approximation (CLA)[12], i.e., the self-consistent combination of the horizontal ladder approximation[13] and the off-diagonal CPA (see also[14]). This scheme given in Section 3 is beyond the RPA-CPA. Stability and damping of the spin waves, Ward relations, and the analogy to the conductivity problem are discussed in Section 4.

2. VERTEX CORRECTIONS TO THE STIFFNESS CONSTANT

Let us handle the itinerant-electron system of narrow-band ferromagnetic alloys A_cB_{1-c} on the basis of the single-band Hubbard Hamiltonian[1] in the random form

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

where $c_{i\sigma}^{+}(c_{i\sigma})$ creates (destroys) a spin σ electron in the Wannier state at lattice site i, and $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$. Within a given alloy configuration $\{\nu\}$ the atomic energy ϵ_i^{ν}

and the bare intra-atomic Coulomb repulsion U_i^{ν} take the random values ϵ^{ν} and U^{ν} ($\nu = A, B$), respectively, according to whether an A- or B- atom occupies the site i. The off-diagonal disorder is assumed to be of the additive type

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

where only nearest-neighbour (n.n.) hopping integrals $t_{ij}^{\nu\mu}$ (or, shortly, $t^{\nu\mu}$) are included.

In the long-wavelength limit the magnon energy $\omega_q = Dq^2$ for cubic crystals can be determined by the spin wave stiffness formula (cf.[4,7,11])

$$D = \frac{1}{n_\uparrow - n_\downarrow}\left[\lim_{q\to 0}\frac{1}{q^2} \ll [S_{\vec{q}}^{+}, qJ_{-\vec{q}}^{-\{\nu\}}] \gg^{\{\nu\}}_{c} - \lim_{\omega\to 0}\lim_{q\to 0} \chi_J^{+-}(\vec{q},\omega)\right] \quad (3)$$

connected with the transverse spin current susceptibility

$$\chi_J^{+-}(\vec{q},\omega) = -\ll\ll J_{\vec{q}}^{+\{\nu\}}, J_{-\vec{q}}^{-\{\nu\}} \gg\gg_{\omega}^{\{\nu\}}{}_{c} \quad (4)$$

Here $(n_\uparrow - n_\downarrow)$ is the average 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. For the model (1) combined with (2) the transverse spin density operator $S_{\vec{q}}^{+}$ (or $S_{-\vec{q}}^{-} = (S_{\vec{q}}^{+})^{+}$) and

its current operator $J^{+}_{\vec{q}}$ (or $J^{-}_{-\vec{q}} = (J^{+}_{\vec{q}})^{+}$) are given by

$$S^{+}_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_i c^{+}_{i\uparrow} c_{i\downarrow} e^{-i\vec{q}\vec{R}_i} , \qquad (5)$$

$$q J^{+\{\nu\}}_{\vec{q}} = q J^{+(0)}_{\vec{q}} + q J^{+(1)\{\nu\}}_{\vec{q}} \qquad (6)$$

with

$$q J^{+(0)}_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_i \sum_j{}' t^{BB} (e^{-i\vec{q}\vec{R}_i} - e^{-j\vec{q}\vec{R}_j}) c^{+}_{i\uparrow} c_{j\downarrow} , \qquad (7)$$

$$q J^{+(1)\{\nu\}}_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_i \sum_j{}' t^{\nu}_{i} (e^{-i\vec{q}\vec{R}_i} - e^{-i\vec{q}\vec{R}_j})(c^{+}_{i\uparrow} c_{j\downarrow} - c^{+}_{j\uparrow} c_{i\downarrow})$$
$$\equiv \sum_i q J^{+(1)\nu}_{\vec{q}\,i} , \qquad (8)$$

where N is the number of lattice sites, $\vec{R}_i$ denotes the position vector of site i, and the prime indicates the summation over nearest neighbours. Note that, contrary to the case of diagonal disorder, the current here includes the random part $J^{+(1)\{\nu\}}_{\vec{q}}$ being additive.

In order to get the stiffness constant D from (3) we are now looking for CPA vertex corrections due to the randomness of the current operator. Start with the first term of (3) rewritten by means of (2), and (5) to (8) as

$$\lim_{q\to 0} \frac{1}{q^2} \ll [\, S^{+}_{\vec{q}} , q J^{-\{\nu\}}_{-\vec{q}} \,] >^{\{\nu\}} >_c = -\frac{1}{6N} \sum_{ij\sigma} \int \frac{dE}{2\pi} < G^{\{\nu\}}_{ij\sigma}(E) \times$$
$$\times \vec{j}^{\,\nu\mu}_{ij}(\vec{R}_i - \vec{R}_j) >_c , \qquad \vec{j}^{\,\nu\mu}_{ij} = -i t^{\nu\mu}_{ij} (\vec{R}_i - \vec{R}_j) , \qquad (9)$$

where $G^{\{\nu\}}_{\sigma}$ is the causal one-particle Green function. Hereafter, the cubic symmetry is employed. The integrand in (9) can be expressed in terms of the one-particle total scattering operator $T^{\{\nu\}}_{\sigma}$ by

$$< \mathrm{tr}\, \{ G^{\{\nu\}}_{\sigma}(z) j^{\{\nu\}'} \} >_c = \mathrm{tr} \{ \mathcal{G}_{\sigma}(z) < j^{\{\nu\}'} >_c \} +$$
$$+ < \mathrm{tr} \{ \mathcal{G}_{\sigma}(z) T^{\{\nu\}}_{\sigma}(z) \mathcal{G}_{\sigma}(z) j^{\{\nu\}'} \} >_c , \qquad j^{\nu\mu'}_{ij} = -i \vec{j}^{\,\nu\mu}_{ij} (\vec{R}_i - \vec{R}_j) , \qquad (10)$$

where the trace means the summation (without spin) over one-particle states, and complex z-arguments refer to the resolvent. Adopting the extended CPA (cf. /12,14/) the averaged propagator $\mathcal{G}_{\sigma}(z) = < G^{\{\nu\}}_{\sigma}(z) >_c$ takes the $\vec{k}$-transform

$$\mathcal{G}_{\vec{k}\sigma}(z) = (z - \epsilon^{B} - t^{BB} s(\vec{k}) - \Sigma_{\sigma}(\vec{k}, z))^{-1} , \qquad (11)$$

where

$$s(\vec{k}) = \sum_{j(\neq i)}{}' e^{i\vec{k}(\vec{R}_i - \vec{R}_j)} . \qquad (12)$$

The coherent self-energy

$$\Sigma_{\sigma}(\vec{k}, z) = \sigma_{0\sigma}(z) + 2\sigma_{1\sigma}(z) s(\vec{k}) + \sigma_{2\sigma}(z) s^2(\vec{k}) \qquad (13)$$

is expressed in terms of $\sigma_{0\sigma}, \sigma_{1\sigma}, \sigma_{2\sigma}$ which satisfy the CPA conditions $< r^{\nu}_{li\sigma} >_c = 0$ ($l = 0, 1, 2$) arising from the constraint $< T^{\nu}_{i\sigma} >_c = 0$ imposed on the single-site scattering matrix

$$\langle \vec{k} | T_{i\sigma}^{\nu} | \vec{k}' \rangle = \frac{1}{N} e^{-i(\vec{k}-\vec{k}')\vec{R}_i} [r_{0i\sigma}^{\nu} + r_{1i\sigma}^{\nu}(s(\vec{k}) + s(\vec{k}')) + r_{2i\sigma}^{\nu} s(\vec{k}) s(\vec{k}')]. \quad (14)$$

The explicit expressions for $r_{1i\sigma}^{\nu}$ are given below.

It is convenient to cast the first term on the r.h.s. of (10) with $\vec{j}^{\{\nu\}}$ from (9) and (2) in the Fourier transform

$$\mathrm{tr}\{\mathcal{G}_{\sigma}(z) \langle j^{\{\nu\}'} \rangle_c\} = -[t^{BB} + c(t^{AA} - t^{BB})] \sum_{\vec{k}} \nabla_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z) \cdot \times \nabla_{\vec{k}} s(\vec{k}), \quad (15)$$

where c denotes the alloy concentration. To evaluate the second contribution of (10) we use the identity (for brevity, (z, σ)-arguments are dropped)

$$\mathrm{tr}\{\mathcal{G} T^{\{\nu\}} \mathcal{G} j^{\{\nu\}'}\} = -[\mathrm{tr}\{\vec{\mathcal{G}}' T^{\{\nu\}} \mathcal{G} j^{\{\nu\}}\} + \mathrm{tr}\{\mathcal{G} T^{\{\nu\}} \vec{\mathcal{G}}' j^{\{\nu\}}\} + \mathrm{tr}\{\mathcal{G} \vec{T}^{\{\nu\}'} \mathcal{G} j^{\{\nu\}}\}]. \quad (16)$$

More explicitly, the "derivatives" in the Wannier space $\vec{\mathcal{G}}'_{ij} = -i\mathcal{G}_{ij}(\vec{R}_i - \vec{R}_j)$ and $\vec{T}_{ij}^{\{\nu\}'} = -iT_{ij}^{\{\nu\}}(\vec{R}_i - \vec{R}_j)$ represent vectors which form scalar products with $j^{\{\nu\}}$ in (16). In averaging (16) the current $j^{\{\nu\}} = j^{(0)} + j^{(1)\{\nu\}}$ can be replaced immediately by its random part $j^{(1)\{\nu\}}$ since the CPA requirement $\langle T^{\{\nu\}} \rangle_c = 0$ holds. Therefore, in the framework of the modified CPA including vertex corrections /14/, it is found that

$$\mathrm{tr}\{\vec{\mathcal{G}}' \langle T^{\{\nu\}} \mathcal{G} j^{(1)\{\nu\}} \rangle_c\} + \mathrm{tr}\{\langle j^{(1)\{\nu\}} \mathcal{G} T^{\{\nu\}} \rangle_c \vec{\mathcal{G}}'\} =$$

$$= \sum_{\vec{k}} [\nabla_{\vec{k}} \Sigma(\vec{k}) - c(t^{AA} - t^{BB}) \nabla_{\vec{k}} s(\vec{k})] \nabla_{\vec{k}} \mathcal{G}_{\vec{k}} . \quad (17)$$

The rest of (16) is handled as follows. The total operator $T^{\{\nu\}}$ can be expressed in terms of T_i^{ν} as multiple scattering series. On the basis of (2) and (9) one decomposes the random current operator into single-site parts through $\vec{j}^{(1)\{\nu\}} = \sum_i \vec{j}^{(1)\nu}_i$. Then the statistical correlations are reduced to

$$\langle \mathrm{tr}\{\mathcal{G} \vec{T}^{\{\nu\}'} \mathcal{G} \vec{j}^{\{\nu\}}\} \rangle_c = \langle \sum_i \mathrm{tr}\{\mathcal{G} \vec{T}_i^{\nu'} \mathcal{G} \vec{j}^{(1)\nu}_i\} \rangle_c , \quad (18)$$

where products of random quantities at the same site are averaged exactly; at different sites, we decouple by factorization, yielding no contribution due to $\langle T_i^{\nu} \rangle_c = 0$ (compare the scheme in /14/).

In the $\vec{k}$-representation we have to substitute

$$\langle \vec{k} | \vec{j}^{(1)\nu}_i | \vec{k}' \rangle = \frac{1}{N} e^{-i(\vec{k}-\vec{k}')\vec{R}_i} t_i^{\nu} (\nabla_{\vec{k}} s(\vec{k}) + \nabla_{\vec{k}'} s(\vec{k}')), \quad (19)$$

$$\langle \vec{k} | \vec{T}_i^{\nu\prime} | \vec{k}' \rangle = \frac{1}{N} e^{-i(\vec{k}-\vec{k}')\vec{R}_i} [r_{1i}^{\nu} (\nabla_{\vec{k}} s(\vec{k}) + \nabla_{\vec{k}'} s(\vec{k}')) +$$

$$+ r_{2i}^{\nu} (s(\vec{k}') \nabla_{\vec{k}} s(\vec{k}) + s(\vec{k}) \nabla_{\vec{k}'} s(\vec{k}'))], \quad (20)$$

and the propagator (11) into (18) leading to

$$\langle \sum_i \mathrm{tr}\{\mathcal{G} \vec{T}_i^{\nu\prime} \mathcal{G} \vec{j}^{(1)\nu}_i\} \rangle_c = 2\sigma_2 \sum_{\vec{k}} \mathcal{G}_{\vec{k}} [\nabla_{\vec{k}} s(\vec{k})]^2, \quad (21)$$

where

$$\sigma_2 = \langle r_{1i}^{\nu} t_i^{\nu} \rangle_c F_0 + \langle r_{2i}^{\nu} t_i^{\nu} \rangle_c F_1 , \qquad (22)$$

$$F_{\ell\sigma}(z) = \frac{1}{N} \sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z)[s(\vec{k})]^{\ell}, \quad (\ell = 0,1,2). \qquad (23)$$

In getting (21) we have used the time-reversal symmetry. The expression (22) for the self-energy part σ_2 (see (13)) has been also derived in the context of the conductivity problem /14/.

Combining (15) to (18) with (21) and recalling the (z,σ)-arguments we obtain the configuration average (10) in the form

$$\langle \mathrm{tr}\{G_{\sigma}^{\{\nu\}}(z) j^{\{\nu\}} \cdot\}\rangle_c = -\sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}^2(z)[\nabla_{\vec{k}}(t^{BB}s(\vec{k}) + \Sigma_{\sigma}(\vec{k},z))^2 - 2\sigma_{2\sigma}(z) \sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z)[\nabla_{\vec{k}} s(\vec{k})]^2 . \qquad (24)$$

Thus the contribution (9) to the stiffness constant D becomes

$$\lim_{q\to 0} \frac{1}{q^2} \ll [S_{\vec{q}}^{+}, qJ_{-\vec{q}}^{-\{\nu\}}] \gg^{\{\nu\}}\rangle_c = \frac{i}{6N} \sum_{\vec{k}\sigma} \int \frac{dE}{2\pi} \{\mathcal{G}_{\vec{k}\sigma}^2(E) \times [\nabla_{\vec{k}}(t^{BB}s(\vec{k}) + \Sigma_{\sigma}(\vec{k},E))]^2 + 2\sigma_{2\sigma}(E)\mathcal{G}_{\vec{k}\sigma}(E)[\nabla_{\vec{k}} s(\vec{k})]^2\} \qquad (25)$$

reexpressed in terms of causal functions.

Extending the microscopic Fermi liquid approach /11/ to off-diagonal disorder the spin current susceptibility (4) reads

$$q^2 \chi_J^{+-}(\vec{q},\omega) = -\frac{i}{N} \int \frac{dE}{2\pi} \langle \mathrm{tr}\{\Lambda_{\uparrow\downarrow}^{\{\nu\}}(E,E+\omega;\vec{q}) \times G_{\downarrow}^{\{\nu\}}(E+\omega)\lambda^{\{\nu\}}(-\vec{q})G_{\uparrow}^{\{\nu\}}(E)\}\rangle_c , \qquad (26)$$

where

$$\Lambda_{\substack{ij \\ \uparrow\downarrow}}^{\{\nu\}}(E,E+\omega;\vec{q}) = \lambda_{ij}^{\nu\mu}(\vec{q}) - \delta_{ij} \int \frac{d\bar{E}}{2\pi} i I_{\substack{i \\ \uparrow\downarrow\downarrow\uparrow}}^{\{\nu\}}(E,\bar{E}+\omega;\omega) \times \sum_{mn} G_{im\uparrow}^{\{\nu\}}(\bar{E}) \Lambda_{\substack{mn \\ \uparrow\downarrow}}^{\{\nu\}}(\bar{E},\bar{E}+\omega;\vec{q}) G_{ni\downarrow}^{\{\nu\}}(\bar{E}+\omega), \qquad (27)$$

$$\lambda_{ij}^{\nu\mu}(\vec{q}) = t_{ij}^{\nu\mu}(e^{-i\vec{q}\vec{R}_i} - e^{-i\vec{q}\vec{R}_j}). \qquad (28)$$

Here only the locality of the irreducible particle-hole vertex $I_{\substack{i \\ \uparrow\downarrow\downarrow\uparrow}}^{\{\nu\}}(E,\bar{E}+\omega;\omega) \equiv I_i^{\{\nu\}}(E,\bar{E}+\omega;E+\omega,\bar{E})$ has been assumed. By expanding $\lambda^{\{\nu\}}$ and the effective spin-flip current $\Lambda_{\uparrow\downarrow}^{\{\nu\}}$ to order $\vec{q}$ in (26), (27), (28) as $\lambda^{\{\nu\}}(\vec{q}) = \vec{q}\cdot\vec{j}^{\{\nu\}}$ and $\Lambda_{\uparrow\downarrow}^{\{\nu\}}(E,E+\omega;\vec{q}) = \vec{q}\cdot\vec{\Lambda}_{\uparrow\downarrow}^{\{\nu\}}(E,E+\omega)$, resp., separating diagonal and off-diagonal parts of $\vec{\Lambda}_{ij}^{\{\nu\}}$, and presuming cubic symmetry one gets

$$\chi_J^{+-}(\vec{q}=0,\omega) = \frac{i}{3N} \int \frac{dE}{2\pi} \langle \mathrm{tr}\{\vec{j}^{\{\nu\}} G_{\downarrow}^{\{\nu\}}(E+\omega) \times \vec{j}^{\{\nu\}} G_{\uparrow}^{\{\nu\}}(E)\}\rangle_c + \tilde{\chi}_J^{+-}(\vec{q}=0,\omega), \qquad (29)$$

where

$$\tilde{\chi}_J^{+-}(\vec{q}=0,\omega) = \frac{i}{3N} \int \frac{dE}{2\pi} \langle \sum_i \vec{\Lambda}_{\substack{ii \\ \uparrow\downarrow}}^{\{\nu\}}(E,E+\omega) \times \vec{K}_{\substack{ii \\ \downarrow\uparrow}}^{\{\nu\}}(E+\omega,E)\rangle_c , \qquad (30)$$

$$\vec{K}_{\substack{ii \\ \downarrow\uparrow}}^{\{\nu\}}(E+\omega,E) = \sum_{mn} G_{im\downarrow}^{\{\nu\}}(E+\omega)\vec{j}_{mn}^{\bar{\mu}\bar{\nu}} G_{ni\uparrow}^{\{\nu\}}(E). \qquad (31)$$

The configurational averaging is achieved in two steps. Since the part (30) affected by electron correlations is beyond the CPA, the first step consists in making the factorization ansatz $\langle \vec{\Lambda}^{\{\nu\}} \cdot \vec{K}^{\{\nu\}} \rangle_c = \langle \vec{\Lambda}^{\{\nu\}} \rangle_c \cdot \langle \vec{K}^{\{\nu\}} \rangle_c$ leading to

$$\langle \vec{K}^{\{\nu\}}_{i\,\downarrow\uparrow}(E+\omega,E)\rangle_c = \frac{1}{N}\sum_{\vec{k}} \mathcal{G}_{\vec{k}\downarrow}(E+\omega)\mathcal{G}_{\vec{k}\uparrow}(E)\,\nabla_{\vec{k}}\Big(t^{BB}s(\vec{k}) + \frac{1}{2}(\Sigma_{\downarrow}(\vec{k},E+\omega)+\Sigma_{\uparrow}(\vec{k},E))\Big) = 0 \qquad (32)$$

and $\tilde{\chi}^{+-}_{J}(\vec{q}=0,\omega)=0$ due to time-reversal symmetry.

In the second step the off-diagonal CPA technique outlined in evaluating (25) can be applied to calculate the vertex corrections for the current-current response in (29) (compare the case treated in /14/), yielding

$$\langle \mathrm{tr}\{\vec{j}^{\{\nu\}}G^{\{\nu\}}_{\downarrow}(E+\omega)\vec{j}^{\{\nu\}}G^{\{\nu\}}_{\uparrow}(E)\}\rangle_c = \sum_{\vec{k}} \mathcal{G}_{\vec{k}\downarrow}(E+\omega)\mathcal{G}_{\vec{k}\uparrow}(E)\times$$

$$\times\Big[\nabla_{\vec{k}}\Big(t^{BB}s(\vec{k}) + \frac{1}{2}(\Sigma_{\downarrow}(\vec{k},E+\omega)+\Sigma_{\uparrow}(\vec{k},E))\Big)\Big]^2 + \qquad (33)$$

$$+\sum_{\vec{k}}[\sigma_{2\downarrow}(E+\omega)\mathcal{G}_{\vec{k}\uparrow}(E)+\sigma_{2\uparrow}(E)\mathcal{G}_{\vec{k}\downarrow}(E+\omega)][\nabla_{\vec{k}}s(\vec{k})]^2.$$

Returning with (25), (29), (30), (32), and (33) to the spin wave stiffness constant (3), we find by performing analytical continuation to retarded "r" quantities the final result

$$D = \frac{1}{6\pi(n_{\uparrow}-n_{\downarrow})}\,\mathrm{Im}\int_{-\infty}^{\mu} dE\,[\Pi^{rr}_{\uparrow\uparrow}(E,E)+\Pi^{rr}_{\downarrow\downarrow}(E,E)-2\Pi^{rr}_{\uparrow\downarrow}(E,E)] \qquad (34)$$

with

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

$$+\Sigma_{\sigma'}(\vec{k},z'))\Big)\Big]^2 + \frac{1}{N}\sum_{\vec{k}}[\sigma_{2\sigma}(z)\mathcal{G}_{\vec{k}\sigma'}(z')+\sigma_{2\sigma'}(z')\mathcal{G}_{\vec{k}\sigma}(z)][\nabla_{\vec{k}}s(\vec{k})]^2,$$

(35)

where the notations $\Pi^{rr}_{\sigma\sigma'}(E,E) \equiv \Pi_{\sigma\sigma'}(E^+,E^+)$, $E^+ = E + i0$ are used. Here the Fermi energy μ is determined from the condition

$$n = \sum_{\sigma} n_{\sigma} = -\frac{1}{\pi}\sum_{\sigma}\int_{-\infty}^{\mu} dE\,\mathrm{Im}\,F^{r}_{0\sigma}(E), \qquad (36)$$

where n is the average number of electrons per site, and $F_{0\sigma}(z)$ is given by (23).

It is pointed out that the compact formulae (34) and (35) for D in ferromagnetic alloys include off-diagonal disorder and electron-electron correlations simultaneously. The nonvanishing vertex corrections originated from the randomness of the spin current are proportional to $\sigma_{1\sigma}$ and $\sigma_{2\sigma}$, i.e., associated with the $\vec{k}$-dependence of the self-energy $\Sigma_{\sigma}(\vec{k},z)$ (13). In particular, a Ward identity is involved in terms of $\nabla_{\vec{k}}\Sigma_{\sigma}(\vec{k},z)$. Restrictions are the additive limit (2) of the off-diagonal randomness and the locality of the kernel $I^{\{\nu\}}_{i\,\uparrow\downarrow\downarrow\uparrow}$ of the Bethe-Salpeter-type equation (27).

3. COHERENT LADDER APPROXIMATION

Next the coherent quantities entering into (34) and (35) are renormalized self-consistently by electron-electron and impurity scattering mechanisms. Within the CLA scheme[12] the local interaction in the particle-particle channel is given in terms of conditionally averaged causal functions by

$$\Sigma^{\nu}_{U\,i\,i\,\sigma}(E) = \int \frac{dE'}{2\pi i}\, G^{\nu}_{i\,i\,-\sigma}(E')\Gamma^{\nu}_{i}(E+E'), \qquad (37)$$

$(\nu = A,B)$

$$\Gamma^{\nu}_{i}(E) = \left[\frac{1}{U^{\nu}_{i}} + \int \frac{dE'}{2\pi i}\, G^{\nu}_{i\,i\,\sigma}(E')G^{\nu}_{i\,i\,-\sigma}(E-E')\right]^{-1}, \qquad (38)$$

where Γ^{ν}_{i} is the effective two-particle vertex. The local Green function $G^{\nu}_{i\,i\,\sigma}(z)$ written as a resolvent is determined in off-diagonal CPA by

$$G^{\nu}_{i\,i\,\sigma}(z) = F_{0\sigma}(z) + F^{2}_{0\sigma}(z) r^{\nu}_{0\,i\,\sigma}(z) + 2F_{0\sigma}(z)F_{1\sigma}(z) r^{\nu}_{1\,i\,\sigma}(z) + F^{2}_{1\sigma}(z) r^{\nu}_{2\,i\,\sigma}(z), \qquad (39)$$

$$\tilde{\epsilon}^{\nu}_{i\sigma}(z) = \delta^{\nu}_{i} + \Sigma^{\nu}_{U\,i\,i\,\sigma}(z), \quad \delta^{\nu}_{i} = \begin{cases} \epsilon^{A} - \epsilon^{B}, & \nu = A \\ 0, & \nu = B, \end{cases} \qquad (40)$$

$$\langle r^{\nu}_{\ell\sigma}(z)\rangle_{c} = \left\langle \frac{a^{\nu}_{\ell\sigma}(z)}{1 - d^{\nu}_{\sigma}(z)} \right\rangle_{c} = 0, \quad (\ell = 0,1,2), \qquad (41)$$

where

$$a^{\nu}_{0\sigma} = (\tilde{\epsilon}^{\nu}_{\sigma} - \sigma_{0\sigma}) + (t^{\nu} - \sigma_{1\sigma})^{2} F_{2\sigma} + (\tilde{\epsilon}^{\nu}_{\sigma} - \sigma_{0\sigma})\sigma_{2\sigma} F_{2\sigma}, \qquad (42)$$

$$a^{\nu}_{1\sigma} = (t^{\nu} - \sigma_{1\sigma}) - (t^{\nu} - \sigma_{1\sigma})^{2} F_{1\sigma} - (\tilde{\epsilon}^{\nu}_{\sigma} - \sigma_{0\sigma})\sigma_{2\sigma} F_{1\sigma}, \qquad (43)$$

$$a^{\nu}_{2\sigma} = -\sigma_{2\sigma} + (t^{\nu} - \sigma_{1\sigma})^{2} F_{0\sigma} + (\tilde{\epsilon}^{\nu}_{\sigma} - \sigma_{0\sigma})\sigma_{2\sigma} F_{0\sigma}, \qquad (44)$$

$$d^{\nu}_{\sigma} = (\tilde{\epsilon}^{\nu}_{\sigma} - \sigma_{0\sigma}) F_{0\sigma} + 2(t^{\nu} - \sigma_{1\sigma}) F_{1\sigma} - \sigma_{2\sigma} F_{2\sigma} - [(t^{\nu} - \sigma_{1\sigma})^{2} + (\tilde{\epsilon}^{\nu}_{\sigma} - \sigma_{0\sigma})\sigma_{2\sigma}][F^{2}_{1\sigma} - F_{0\sigma} F_{2\sigma}]. \qquad (45)$$

Here the atomic potential $\tilde{\epsilon}^{\nu}_{i\sigma}(z)$ is energy-dependent through the self-energy $\Sigma^{\nu}_{U\,i\,i\sigma}(z)$ caused by electron correlations, t^{ν}_{i} is given in (2) (i indices are dropped in (41) to (45)), and $F_{\ell\sigma}$ is defined by (23). The CPA conditions (41) are averaged configurationally with weights c and (1-c). By combining (36) to (45) with (23) and (11), (12), (13) to a self-consistency loop we make available the quantities needed to compute the stiffness constant D from (34) via (35).

Let us pass to some limiting cases:

(i) In the Hartree-Fock approximation one gets, instead of (37) and (38), the constant self-energy $\Sigma^{\nu\,HF}_{U\,i\,i\sigma} = U^{\nu}_{i}\, n^{\nu}_{i-\sigma}$, where $n^{\nu}_{i\sigma}$ denotes the average electron number with spin σ at ν-sites given by

$$n_{i\sigma}^{\nu} = -\frac{1}{\pi}\int_{-\infty}^{\mu} dE\, \mathrm{Im} G_{ii\sigma}^{r\nu}(E). \qquad (46)$$

Otherwise, the present scheme remains to be unaltered.

(ii) In the case of only diagonal disorder (labeled by d), i.e., $t_i^{\nu} = 0$ and $\sigma_1 = \sigma_2 = 0$, (39) takes the form

$$G_{ii\sigma}^{\nu}(z) = \frac{F_{0\sigma}(z)}{1-(\tilde{\epsilon}_{i\sigma}^{\nu}(z)-\sigma_{0\sigma}(z))F_{0\sigma}(z)} \qquad (47)$$

and (41) can be reduced to the CPA condition

$$\langle r_{0\sigma}^{\nu}(z)\rangle_c = \left\langle \frac{\tilde{\epsilon}_{\sigma}^{\nu}(z)-\sigma_{0\sigma}(z)}{1-(\tilde{\epsilon}_{\sigma}^{\nu}(z)-\sigma_{0\sigma}(z))F_{0\sigma}(z)} \right\rangle_c = 0. \qquad (48)$$

Note that the $\vec{k}$-independent coherent potential $\Sigma_{\sigma}(z) \equiv \sigma_{0\sigma}(z)$ may be redefined by $\Sigma_{\sigma}(z) = \epsilon^{B} + \sigma_{0\sigma}(z)$ according to[11]. The stiffness constant in (34) and (35) becomes

$$D_d = \frac{1}{6\pi(n_{\uparrow}-n_{\downarrow})}\mathrm{Im}\int_{-\infty}^{\mu} dE \frac{1}{N}\sum_{\vec{k}}(\mathcal{G}_{\vec{k}\uparrow}^{r}(E)-\mathcal{G}_{\vec{k}\downarrow}^{r}(E))^2(\nabla_{\vec{k}}\epsilon_{\vec{k}})^2, \qquad (49)$$

where $\epsilon_{\vec{k}} = t^{BB}s(\vec{k})$. The horizontal ladder approximation (37) and (38) is retained.

(iii) By restricting ourselves to both the Hartree-Fock approximation and diagonal disorder we arrive at the RPA-CPA result[3 to 7] having the form (49) related to the case (i).

4. VALIDITY CONSIDERATION

Consider now some additional points which contribute to the justification of the present approach. Using (5) one can introduce the transverse susceptibility (cf.[11])

$$\chi^{+-}(\vec{q},\omega) = -\langle\langle S_{\vec{q}}^{+}, S_{-\vec{q}}^{-}\rangle\rangle_{\omega}^{\{\nu\}}\rangle_c = \frac{i}{N}\int\frac{dE}{2\pi}\langle \mathrm{tr}\{\Lambda_{0\uparrow\downarrow}^{\{\nu\}}(E,E+\omega;\vec{q})\times G_{\downarrow}^{\{\nu\}}(E+\omega)\lambda_0(-\vec{q})G_{\uparrow}^{\{\nu\}}(E)\}\rangle_c , \qquad (50)$$

where the effective spin-flip density $\Lambda_{0\uparrow\downarrow}^{\{\nu\}}$ obeys an integral equation analogous to (27) with $\lambda_{ij}^{\nu\mu}(\vec{q})$ replaced by $\lambda_{0ij}(\vec{q}) = e^{-i\vec{q}\vec{R}_i}\delta_{ij}$. Taking into account the special vertex

$$I_{i\ \uparrow\downarrow\downarrow\uparrow}^{\{\nu\}}(E,\bar{E}+\omega;\omega) = -\Gamma_{i\ \uparrow\downarrow\downarrow\uparrow}^{\{\nu\}}(E+\bar{E}+\omega) \equiv -\Gamma_i^{\{\nu\}}(E+\bar{E}+\omega),$$

the equation (27) and its analog for $\Lambda_{0\uparrow\downarrow}^{\{\nu\}}$ combined with (37) and (38) in the completely random version (i.e., ν replaced by $\{\nu\}$) yield

$$\omega\Lambda_{0i\ \uparrow\downarrow}^{\{\nu\}}(E,E+\omega;\vec{q})\delta_{ij} - \Lambda_{ij\ \uparrow\downarrow}^{\{\nu\}}(E,E+\omega;\vec{q}) = e^{-i\vec{q}\vec{R}_i}G_{ij\downarrow}^{\{\nu\}-1}(E+\omega) - G_{ij\uparrow}^{\{\nu\}-1}(E)e^{-i\vec{q}\vec{R}_j}, \qquad (51)$$

where

$$(G^{\{\nu\}-1}(E))_{ij\sigma} = (E-\epsilon_i^{\nu})\delta_{ij} - t_{ij}^{\nu\mu} - \Sigma_{Uii\sigma}^{\{\nu\}}(E)\delta_{ij}. \qquad (52)$$

The Ward-Takahashi-type relation (51) refers to a spin conserving approximation within the configuration $\{\nu\}$.

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

$$\hat{D} = D(n_{\uparrow}-n_{\downarrow}) > 0 \qquad (53)$$

may be found from the spectral representation

$$\chi^{+-r}(\vec{q},\omega) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{\mathrm{sign}\,\omega'}{\omega-\omega'+i\epsilon}\,\hat{I}_{S^+_{\vec{q}}S^-_{-\vec{q}}}(\omega'), \quad (54)$$

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

$$\chi^{+-r}_{\mathrm{pole}}(\vec{q},\omega) = -\frac{n_\uparrow - n_\downarrow}{\omega - Dq^2 + i\epsilon} \quad (55)$$

can be separated for small q and ω from the Stoner continuum, because the individual excitations of the electron-hole pairs have vanishing spectral weight for $\vec{q}\to 0$. Note that the expression (55) implies a Goldstone boson characterized by $\lim_{q\to 0}\omega_q = 0$ arising from the breakdown (through $n_\uparrow \neq n_\downarrow$) of the spin rotational invariance which is given by $[H^{\{\nu\}}, S^+_{\vec{q}=0}] = 0$ with $H^{\{\nu\}}$ from (1). The comparison of (54) and (55) leads to (53).

In the present approximation the spin wave damping γ_q, which enters into (55) instead of $\epsilon\to 0$, can be proved to be

$$\gamma_q = \frac{q^2}{n_\uparrow - n_\downarrow}\,\mathrm{Im}\,\chi^{+-r}_J(0,Dq^2) = \quad (56)$$

$$= \frac{Dq^4}{6\pi(n_\uparrow - n_\downarrow)}\,\mathrm{Re}\{\Pi^{ra}_{\uparrow\downarrow}(\mu,\mu) - \Pi^{rr}_{\uparrow\downarrow}(\mu,\mu)\},$$

where $\Pi^{ra}_{\uparrow\downarrow}(\mu,\mu) \equiv \Pi_{\uparrow\downarrow}(\mu^+,\mu^-)$ and $\Pi^{rr}_{\uparrow\downarrow}(\mu,\mu)$ are available from (35), and $\mu^- = \mu - i0$. For the case without off-diagonal disorder, (56) simplifies to [11]

$$\gamma_{qd} = \frac{D_d q^4}{3\pi(n_\uparrow - n_\downarrow)N}\sum_{\vec{k}}\mathrm{Im}\,\mathcal{G}^r_{\vec{k}\uparrow}(\mu)\,\mathrm{Im}\,\mathcal{G}^r_{\vec{k}\downarrow}(\mu)(\nabla_{\vec{k}}\epsilon_{\vec{k}})^2 \quad (57)$$

corresponding to the RPA-CPA result [5].

It should be mentioned that the longitudinal electrical conductivity can be calculated with the same accuracy as D. In doing so, the dissipative part of the scalar ac conductivity $\mathrm{Re}\,\sigma^r(\omega)$ is obtained as a generalized Kubo-Greenwood formula

$$\mathrm{Re}\,\sigma^r(\omega) = \frac{e^2N}{12\pi V}\sum_\sigma\int dE\left(\frac{f(E)-f(E+\omega)}{\omega}\right)\times$$

$$\times[\Pi^{ra}_{\sigma\sigma}(E+\omega,E)+\Pi^{ar}_{\sigma\sigma}(E+\omega,E)-\Pi^{rr}_{\sigma\sigma}(E+\omega,E)-\Pi^{aa}_{\sigma\sigma}(E+\omega,E)], \quad (58)$$

where $f(E) = \Theta(\mu - E)$ is the Fermi function at zero temperature, V is the volume of the system, and e denotes the electronic charge. In the static limit one deduces from (58) the dc conductivity $\sigma = \sigma^r(\omega = 0)$ as

$$\sigma = \frac{e^2N}{6\pi V}\sum_\sigma[\Pi^{ra}_{\sigma\sigma}(\mu,\mu) - \mathrm{Re}\,\Pi^{rr}_{\sigma\sigma}(\mu,\mu)] \equiv \sum_\sigma \sigma_\sigma\,. \quad (59)$$

Here $\Pi^{ra}_{\sigma\sigma}(E+\omega,E) = \Pi_{\sigma\sigma}(E^+ + \omega, E^-)$, etc., are given in (35), and the conductivities $\sigma_{\uparrow(\downarrow)}$ for $\uparrow(\downarrow)$ spin electrons indicate the ferromagnetic state. For diagonal disorder there follows the conventional form

$$\sigma_d = \frac{e^2}{3\pi V_{\vec{k}\sigma}} \sum [\operatorname{Im} \mathcal{G}^r_{\vec{k}\sigma}(\mu)]^2 \, (\nabla_{\vec{k}} \epsilon_k)^2. \qquad (60)$$

Note that the Green functions and self-energies in (58), (59), and (60) are renormalized by electron correlations within the CLA.

5. CONCLUSION

The present derivation of a renormalized spin wave stiffness constant of ferromagnetic metallic alloys involves CPA vertex corrections of the spin current susceptibility due to random transfer integrals of the special type $t^{AB} = \frac{1}{2}(t^{AA} + t^{BB})$. This additive limit seems to be reasonable, e.g., for dilute ferromagnets (cf. /15/ and references therein and makes also contact to bond-type disordered systems. Another current vertex correction has been excluded a priori by assuming locality of the effective four-leg vertices originated from the random Hubbard term. Such a zero range interaction can be justified by the screening effect of the (otherwise ignored) s electrons in the metal. The spin wave treatment is confirmed by a stability criterion, small damping at least of order q^4, and the fulfilment of Ward identities. According to the horizontal ladder approximation the proposed scheme is suitable for strong electron correlations and small carrier densities as realized, e.g., in some Ni-based alloys. Numerical results of self-consistent calculations will be reported in a subsequent paper.

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Received by Publishing Department
on October 16 1978.