INFLUENCE OF ORDERING ON THE SPIN WAVE STIFFNESS CONSTANT IN ITINERANT ELECTRON FERROMAGNETIC TRANSITION METAL ALLOYS*

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An expression for the spin wave stiffness constant in a partially long range ordered ferromagnetic alloy is derived for a four-sublattice model using the random phase approximation and the coherent potential approximation. Both the "average exchange" and the "magnon scattering" terms are included.

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1. Introduction

Neutron inelastic scattering results on Ni_3Fe by Mikke et al. [1] indicate that the influence of atomic ordering on the magnon energy is significant. Similar behaviour was also investigated by Menzinger et al. [2] on Pd_3Fe.

Previous works on partially long range ordered alloys, using the itinerant electron picture, were by Morkowski [3] and Takahashi and Edwards [6]. Morkowski's approach is a perturbational one, where the departures from stoichiometry and from full order are taken as small parameters. In this limit magnons for a complete ordered alloy serve as a good starting point in the description of magnon scattering. In Takahashi and Edwards' method the acoustic magnon energy is found from the poles of averaged over sublattices transverse susceptibility for the single-site CPA effective medium Hamiltonian. Although the only experimental data are for Ni_3Fe and Pd_3Fe in both theoretical articles referred to above an alloy of b.c.c. structure of composition $A_{0.5}B_{0.5}$ or close to it was considered.

In the present paper a method for calculating the spin wave stiffness constant in a four-sublattice system is developed. Both the "average exchange" contribution, which reflects the changes of the electronic structure of the ground state and the "magnon scattering" due to the random deviations from effective medium potentials are taken into account.

The remainder of the paper is organized as follows. In Section 2 the CPA equations to determine the coherent potentials are derived. In Section 3 the acoustic magnon opera-

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tors for an effective CPA medium are determined. In terms of these operators an effective magnon Hamiltonian [4] is set up in Section 4. Finally the magnon energy is determined from the poles of the magnon Green functions averaged over configurations by the method of Kaneyoshi [7].

2. *Model Hamiltonian and CPA equations*

We consider a stoichiometric binary alloy AB_3. In the model to be used it is assumed that the lattice may be divided into four equivalent s.c. sublattices. Three of them are occupied by atoms B with equal probability, hereafter denoted by p, whereas for the fourth sublattice this probability, in general, differs and can be expressed in terms of the parameter p as $3(1-p)$. Retaining the essential features, we may significantly simplify our problem by assuming that the Fourier transforms of the hopping integrals between any of the two different sublattices are the same. Let us write the model Hamiltonian as the sum of two terms, an effective medium Hamiltonian H_0 with effective potentials determined in the single-site CPA and the perturbation V due to the local deviations from effective potentials.

$$H = H_0 + V, \tag{1}$$

H_0 is a configuration independent part and reads

$$H_0 = \sum_{k\lambda\sigma} t_\lambda(\omega) a^\dagger_{\lambda k\sigma} a_{\lambda k\sigma} + \sum_{k\sigma} \sum_{\lambda \neq \lambda'} t z_k a^\dagger_{\lambda k\sigma} a_{\lambda' k\sigma}$$
$$+ \sum_{\substack{k\lambda \\ k' q_1}} \frac{4 I_\lambda(\omega)}{N} a^\dagger_{\lambda k+q_1 +} a^\dagger_{\lambda k'-q_1 -} a_{\lambda k'-} a_{\lambda k+}, \tag{2}$$

where $a^\dagger_{\lambda k\sigma}$ is the creation operator in the Bloch state on sublattice λ ($\lambda = 1, 2, 3, 4$). N is the number of all lattice sites. The effective atomic potentials $t_\lambda(\omega)$ and the intraatomic Coulomb integrals $I_\lambda(\omega)$ will be determined later by (21) and (22) in the single-site CPA. According to the model assumptions

$$(t_\lambda(\omega), I_\lambda(\omega)) = \begin{cases} (t_A(\omega), I_A(\omega)) & \text{for} \quad \lambda = 1 \\ (t_B(\omega), I_B(\omega)) & \text{for} \quad \lambda = 2, 3, 4. \end{cases} \tag{3}$$

The Fourier transform of the nearest neighbours hopping integral t is taken in the form tz_k, where

$$z_k = \tfrac{1}{3} \sum_\delta \exp(i\boldsymbol{k} \cdot \boldsymbol{\delta}), \tag{4}$$

where $\boldsymbol{\delta}$ runs over nearest neighbours in the f.c.c. lattice. The configuration dependent part of our Hamiltonian is

$$V = \sum_{\alpha\lambda} \sum_{kk'\sigma} [t_\alpha - t_\lambda(\omega)] \varphi_{\alpha\lambda}(k-k') a^\dagger_{\lambda k\sigma} a_{\lambda k'\sigma}$$
$$+ \frac{4}{N} \sum_{\alpha\lambda} \sum_{k_1,k_2,k_3,k_4} [I_\alpha - I_\lambda(\omega)] \varphi_{\alpha\lambda}(k_1 + k_3 - k_2 - k_4) a^\dagger_{\lambda k_1 +} a^\dagger_{\lambda k_3 -} a_{\lambda k_4 -} a_{\lambda k_2 +}. \tag{5}$$

The subscript α takes the values 1 and 2 denoting atoms A and B respectively.

$$\varphi_{\alpha\lambda}(k) = \frac{4}{N}\sum_{i_\lambda} c_i^{\alpha\lambda} \exp(i\boldsymbol{k}\cdot\boldsymbol{i}_\lambda) \tag{6}$$

and the random variables $c_i^{\alpha\lambda}$ are defined as follows

$$c_i^{\alpha\lambda} = \begin{cases} 1 & \text{if the lattice site } i_\lambda \text{ is occupied by atom } \alpha \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

The time Fourier transform $G_{\lambda\lambda_1,\sigma}(k,\omega)$ of the retarded Green function $\langle\langle a_{\lambda k\sigma}(t); a^\dagger_{\lambda_1 k\sigma}\rangle\rangle$ for the system described by Hamiltonian H_0 satisfies the following equation of motion in the Hartree–Fock approximation

$$[\omega - \Sigma_{\lambda\sigma}(\omega)]G_{\lambda\lambda_1,\sigma}(k,\omega) - \sum_{\gamma\neq\lambda} tz_k G_{\gamma\lambda_1,\sigma}(k,\omega) = \delta_{\lambda\lambda_1}, \tag{8}$$

where

$$\Sigma_{\lambda\sigma}(\omega) = t_\lambda(\omega) + I_\lambda(\omega)\langle n_{\lambda-\sigma}\rangle, \tag{9}$$

and $\langle n_{\lambda\sigma}\rangle = \langle a^\dagger_{\lambda i\sigma} a_{\lambda i\sigma}\rangle$. We get the following solutions:

$$G_{\lambda\lambda,\sigma}(k,\omega) = \frac{A_{\lambda\sigma}(k,\omega)}{B_{\lambda\sigma}(k,\omega)}, \tag{10}$$

with

$$\begin{aligned} A_{1\sigma}(k,\omega) &= \omega - \Sigma_{2\sigma}(\omega) - 2tz_k \\ B_{1\sigma}(k,\omega) &= [\omega-\Sigma_{1\sigma}(\omega)][\omega-\Sigma_{2\sigma}(\omega)] - 2tz_k[\omega-\Sigma_{1\sigma}(\omega)] - 3t^2z_k^2, \end{aligned} \tag{11}$$

and for $\lambda = 2, 3, 4$

$$\begin{aligned} A_{\lambda\sigma}(k,\omega) &= [\omega-\Sigma_{1\sigma}(\omega)][\omega-\Sigma_{2\sigma}(\omega)] - tz_k[\omega-\Sigma_{1\sigma}(\omega)] - 2t^2z_k^2 \\ B_{\lambda\sigma}(k,\omega) &= [\omega-\Sigma_{2\sigma}(\omega)]^2[\omega-\Sigma_{1\sigma}(\omega)] - tz_k[\omega-\Sigma_{2\sigma}(\omega)][\omega-\Sigma_{1\sigma}(\omega)] \\ &\quad - t^2z_k^2[5\omega - 3\Sigma_{2\sigma}(\omega) - 2\Sigma_{1\sigma}(\omega)] - 3t^3z_k^3. \end{aligned} \tag{12}$$

The coherent potentials are determined by the requirement that the configuration average of the t matrix for scattering from a single site on sublattice λ should vanish (cf. [8]). Namely,

$$\langle c_i^{\alpha\lambda}\rangle\{[\varepsilon_{\alpha\lambda\sigma} - \Sigma_{\lambda\sigma}(\omega)]^{-1} - F_{\lambda\sigma}(\omega)\}^{-1} + \langle c_i^{\bar{\alpha}\lambda}\rangle\{[\varepsilon_{\bar{\alpha}\lambda\sigma} - \Sigma_{\lambda\sigma}(\omega)]^{-1} - F_{\lambda\sigma}(\omega)\}^{-1} = 0 \tag{13}$$

with

$$\varepsilon_{\alpha\lambda\sigma} = t_\alpha + I_\alpha\langle n_{\alpha\lambda-\sigma}\rangle, \tag{14}$$

where t_α and I_α are atomic potential for atom α and intraatomic potential respectively, $\bar{\alpha}$ denotes the opposite atom from atom α and $\langle n_{\alpha\lambda\sigma}\rangle$ is the occupation of electrons with

spin σ on the atom α, if this atom occupies the site of sublattice λ. The definition of the function $F_{\lambda\sigma}(\omega)$ is

$$F_{\lambda\sigma}(\omega) = \frac{4}{N}\sum_{k} G_{\lambda\lambda,\sigma}(k, \omega). \tag{15}$$

Note that, as a consequence of our model assumptions, the only independent equations (13) are for $\lambda = 1, 2$. The configurational averages $\langle c_i^{\alpha\lambda}\rangle$ are connected with the long range order parameter p by the relations

$$\langle c_i^{11}\rangle = 3p-2; \qquad \langle c_i^{12}\rangle = 1-p$$
$$\langle c_i^{21}\rangle = 3(1-p); \qquad \langle c_i^{22}\rangle = p. \tag{16}$$

Having in mind that CPA is a self-consistent method, it is convenient for numerical analysis to replace the summations over $\boldsymbol{k}$ space by one dimensional integration. Observing that the Green functions (10) are functions of z_κ (4) only it is useful to introduce the function $N(\varepsilon)$ defined by the integral

$$N(\varepsilon) = \frac{v}{(2\pi)^3}\int_{z_k=\varepsilon}\frac{ds}{|\nabla z_k|}, \tag{17}$$

where the integration extends over the surface of constant value z_k and v is the volume of the elementary cell. Now we can rewrite (15) as follows

$$F_{\lambda\sigma}(\omega) = \int d\varepsilon N(\varepsilon) G_{\lambda\lambda,\sigma}(\varepsilon, \omega). \tag{18}$$

The total density of electron states with spin σ is given by

$$\varrho_\sigma(E) = -\frac{1}{4\pi}[\operatorname{Im} F_{1\sigma}(E+i\delta)+3\operatorname{Im} F_{2\sigma}(E+i\delta)]. \tag{19}$$

Similarly, the conditional local densities of states $\varrho_{\alpha\lambda\sigma}(E)$ i.e. the density of states of electrons with spin σ on the site belonging to sublattice λ, if this site is occupied by an atom α, can be expressed by

$$\varrho_{\alpha\lambda\sigma}(E) = -\frac{1}{\pi}\{\operatorname{Im} F_{\lambda\sigma}(E+i\delta)^{-1}-[\varepsilon_{\alpha\lambda\sigma}-\Sigma_{\lambda\sigma}(E+i\delta)]\}^{-1}. \tag{20}$$

To complete the set of coupled equations let us write the standard formula for the electron occupation numbers

$$n_{\alpha\lambda\sigma} = \int_{-\infty}^{E_F} dE\varrho_{\alpha\lambda\sigma}(E). \tag{21}$$

All the quantities $\Sigma_{\lambda\sigma}(\omega)$, $n_{\alpha\lambda\sigma}$ and E_F must be determined self-consistently through equations (10), (13), (18) and (21). Using equations (9) we can write the effective atomic potentials

and the effective intraatomic Coulomb integrals in the form:

$$t_\lambda(\omega) = \Sigma_{\lambda\sigma}(\omega) - \frac{[\Sigma_{\lambda\sigma}(\omega)-\Sigma_{\lambda-\sigma}(\omega)]\langle n_{\lambda-\sigma}\rangle}{\langle n_{\lambda-\sigma}\rangle - \langle n_{\lambda\sigma}\rangle}, \tag{22}$$

$$I_\lambda(\omega) = \frac{\Sigma_{\lambda\sigma}(\omega)-\Sigma_{\lambda-\sigma}(\omega)}{\langle n_{\lambda-\sigma}\rangle - \langle n_{\lambda\sigma}\rangle}. \tag{23}$$

3. Magnons in the effective medium

Let us assume that Hamiltonian H_0 has a ferromagnetic ground state. We can define the magnon creation operator as follows

$$\beta^\dagger_{qr} = \sum_{ps\mu} b^r_{s\mu}(p+q, p; \omega) a^\dagger_{p+qs+} a_{p\mu-}. \tag{24}$$

Here indices s, μ label sublattices, whereas index r stands for different branches of magnon spectrum. Because of the ω dependence the above definition differs from the usual one for pure metals. For the sake of brevity we shall not write ω explicitly in further formulas. The magnon amplitudes $b^r_{s\mu}(p+q, p)$ and the magnon energy are calculated by solving in RPA the equation of motion for $\beta^\dagger_{qr}$ with Hamiltonian H_0. We get the following set of equations

$$(\Omega_{s\mu}-E_q)b_{s\mu}(p+q, p) + \sum_{\lambda\neq s} tz_{p+q} b_{\lambda\mu}(p+q, p) - \sum_{\lambda\neq\mu} tz_p b_{s\lambda}(p+q, p)$$

$$+\delta_{s\mu}\frac{4I_s}{N}\sum_k (n_{k+qs+}-n_{ks-})b_{ss}(k+q, k) = 0, \tag{25}$$

where

$$\Omega_{s\mu} = t_s - t_\mu + I_s n_{s-} - I_\mu n_{\mu+}. \tag{26}$$

Due to the symmetry of H_0 the amplitudes of the acoustical magnons satisfy the following relations:

$$\begin{aligned}
&b_{12}(p+q, p) = b_{13}(p+q, p) = b_{14}(p+q, p),\\
&b_{21}(p+q, p) = b_{31}(p+q, p) = b_{41}(p+q, p),\\
&b_{23}(p+q, p) = b_{32}(p+q, p) = b_{34}(p+q, p) = b_{43}(p+q, p) = b_{24}(p+q, p)\\
&\qquad\qquad = b_{42}(p+q, p),\\
&b_{22}(p+q, p) = b_{33}(p+q, p) = b_{44}(p+q, p).
\end{aligned} \tag{27}$$

In a semiclassical picture the above symmetry relations can be interpreted as the reflection of "in-phase motion" of spins on different sublattices. In all considerations to follow we

shall be concerned only with acoustical magnons. From (25) using (27) we get equation (28) determining in RPA the acoustic magnon energy spectrum

$$\det\left[\Gamma_{\lambda r}(q, E_q)-\delta_{\lambda r}\right] = 0. \tag{28}$$

Here the subscripts λ, r take the values 1, 2 and

$$\Gamma_{\lambda r}(q, E_q) = \frac{4I_r}{N}\sum_p L_{\lambda r}(p+q, p, E_q)\,(n_{p\lambda -}-n_{p+q\lambda +}), \tag{29}$$

with

$$L_{\lambda r}(p+q, p, E_q) = \frac{(-1)^{\lambda+r}M_{\lambda r}(p+q, p, E_q)}{\det\left[M_{ij}(p+q, p, E_q)\right]}, \tag{30}$$

where

$$M_{11}(p+q, p, E_q) = \Omega_{22}-E_q-t^2\left(\frac{z_{p+q}^2}{c}+\frac{z_p^2}{R}\right)$$

$$+v_{23}\left[2t(z_{p+q}-z_p)-2t^2\left(\frac{z_{p+q}^2}{c}+\frac{z_p^2}{R}\right)\right],$$

$$M_{12}(p+q, p, E_q) = 3t^2(2v_{23}+1)z_{p+q}z_p\left(\frac{1}{c}+\frac{1}{R}\right),$$

$$M_{21}(p+q, p, E_q) = t^2 z_{p+q}z_p\left(\frac{1}{c}+\frac{1}{R}\right)+u_{23}\left[2t(z_{p+q}-z_p)-2t^2\left(\frac{z_{p+q}^2}{c}+\frac{z_p^2}{R}\right)\right],$$

$$M_{22}(p+q, p, E_q) = \Omega_{11}-E_q-3t^2\left(\frac{z_p^2}{c}-\frac{z_{p+q}^2}{R}\right)+6t^2u_{23}z_{p+q}z_p\left(\frac{1}{c}+\frac{1}{R}\right), \tag{31}$$

where the following abbreviations were introduced

$$c = \Omega_{12}-2tz_p-E_q,$$

$$R = \Omega_{21}+2tz_{p+q}-E_q, \tag{32}$$

and u_{23}, v_{23} are given below together with two other pairs of coefficients, which will be used later (see (36))

$$u_{23} = \frac{-t^2 z_{p+q}z_p\left(\frac{1}{c}+\frac{1}{R}\right)}{\Omega_{22}-E_q+t(z_{p+q}-z_p)-2t^2\left(\frac{z_{p+q}^2}{c}+\frac{z_p^2}{R}\right)},$$

$$v_{23} = \frac{t^2\left(\frac{z_{p+q}^2}{c}+\frac{z_p^2}{R}\right)-t(z_{p+q}-z_p)}{\Omega_{22}-E_q+t(z_{p+q}-z_p)-2t^2\left(\frac{z_{p+q}^2}{c}+\frac{z_p^2}{R}\right)},$$

$$u_{12} = \frac{t}{c}(z_p - 2z_{p+q}u_{23}), \quad v_{12} = \frac{-tz_{p+q}}{c}(1+2v_{23}),$$

$$u_{21} = -\frac{t}{R}(z_{p+q} - 2u_{23}z_p), \quad v_{21} = \frac{tz_p}{R}(1+2v_{23}). \tag{33}$$

The magnon amplitudes corresponding to the solution of equation (28) are

$$b_{s\mu}(p+q, p) = d_q B_{s\mu}(p+q, p), \tag{34}$$

where d_q is the normalization factor and

$$B_{s\mu}(p+q, p) = \frac{4I_A}{N} L_{s1}(p+q, p, E_q) + \frac{4I_B}{N} L_{s2}(p+q, p, E_q) \frac{\Gamma_{11}(q, E_q) - 1}{\Gamma_{12}(q, E_q)} \tag{35}$$

for $(s, \mu) \in \{(1,1), (2,2)\}$, and

$$B_{s\mu}(p+q, p) = u_{s\mu}B_{11}(p+q, p) + v_{s\mu}B_{22}(p+q, p) \tag{36}$$

for $(s, \mu) \in \{(1, 2), (2, 1), (2, 3)\}$.

It is convenient to choose the normalization factor d_q in such a way that operators β_q, $\beta_{q'}^{\dagger}$ satisfy in RPA the Bose commutation rules $\langle[\beta_q, \beta_{q'}^{\dagger}]\rangle = \delta_{qq'}$.

By an expansion of (28) up to terms proportional to q squared one gets, employing cubic symmetry, the spin wave stiffness constant in the form

$$D_{\text{Av.exch.}} = \frac{\sum_{s,\mu} [\delta_{s\mu} - (-1)^{s+\mu}\Gamma_{s\mu}(0, 0)] [F_{\bar{s}\bar{\mu}} + G_{\bar{s}\bar{\mu}}]}{\sum_{s,\mu} [\delta_{s\mu} - (-1)^{s+\mu}\Gamma_{s\mu}(0, 0)] \frac{4I_{\bar{\mu}}}{N} \sum_p L_{\bar{s}\bar{\mu}}^{(3)}(p) (n_{p\bar{s}+} - n_{p\bar{s}-})}, \tag{37}$$

where the indices s, μ, $\bar{s}$, $\bar{\mu}$ take the values 1, 2 but $s \neq \bar{s}$ and $\mu \neq \bar{\mu}$

$$F_{s\mu} = \frac{2I_\mu}{3N} \sum_p [L_{s\mu}^{(1)}(p) (n_{ps-} - n_{ps+}) - L_{s\mu}^{(0)}(p) n_{ps+}^{(1)}] \nabla^2 z_p,$$

$$G_{s\mu} = \frac{4I_\mu}{3N} \sum_p \{[L_{s\mu}^{(2)}(p) - L_{s\mu}^{(1)}(p)] (n_{ps-} - n_{ps+}) - L_{s\mu}^{(0)} n_{ps+}^{(2)}\} |\nabla z_p|^2. \tag{38}$$

The quantities $L_{s\mu}^{(t)}(p)$ are defined as follows

$$L_{s\mu}^{(0)}(p) = L_{s\mu}(p, p, 0),$$

$$L_{s\mu}^{(1)}(p) = \frac{\partial}{\partial z_{p+q}} L_{s\mu}(p+q, p, E_q)|_{q=0},$$

$$L^{(2)}_{s\mu}(p) = \frac{\partial^2}{\partial z^2_{p+q}} L_{s\mu}(p+q, p, E_q)|_{q=0},$$

$$L^{(3)}_{s\mu}(p) = \frac{\partial}{\partial E_q} L_{s\mu}(p+q, p, E_q)|_{q=0}. \tag{39}$$

Replacing $L_{s\mu}(p+q, p, E_q)$ in (39) by $n_{p+qs\sigma}$ one can obtain the definitions of $n^{(t)}_{ps\sigma}$.

Following Edwards and Fung [9] we call the contribution to the spin wave stiffness constant represented by the formula (37) the "average exchange" contribution. This name reflects the fact that (37) corresponds to the acoustic magnon propagating in the average medium (in the case under consideration — in the medium determined in the single-site CPA). As it is well known in the single-site CPA one requires that a single scatterer imbedded in the effective medium should produce no further scattering on the average [8]. The vanishing of electron single-site t matrix however does not imply vanishing of average magnon t matrix. To improve the description of our problem it is necessary to include magnon scattering terms. This is the aim of the next Section.

4. Magnon scattering

The renormalization of the magnon energy due to the magnon scattering processes can be found by a simple generalization of the method described by Morkowski in [3, 5]. It is very useful to set up the effective magnon Hamiltonian [4] in terms of magnon creation and destruction operators $\beta^\dagger_q$, β_q defined in the preceding Section (24), (34–36). For the present purpose only bilinear terms in the effective Hamiltonian are needed, thus

$$H_{\text{eff}} = \sum_{qq'} A(q, q')\beta^\dagger_q \beta_{q'}, \tag{40}$$

where

$$A(q, q') = \langle 0|\, [\beta_q, [H, \beta^\dagger_{q'}]]\, |0\rangle, \tag{41}$$

and $|0\rangle$ denotes the ground state of H_0. Calculations give

$$A(q, q') = E^0_q \delta_{qq'} + \sum_{\alpha\lambda} \varphi_{\alpha\lambda}(q-q') T_{\alpha\lambda}(q, q'), \tag{42}$$

E^0_q is the energy of magnons for an effective medium and

$$T_{\alpha\lambda}(q, q') = [t_\alpha - t_\lambda(\omega)] f_\lambda(q, q') + [I_\alpha - I_\lambda(\omega)] h_\lambda(q, q'), \tag{43}$$

with

$$f_\lambda(q, q') = \sum_{p\mu} b^*_{\lambda\mu}(p+q, p) b_{\lambda\mu}(p+q', p)\,(n_{p\mu-} - n_{p+q\lambda+})$$

$$- b^*_{\mu\lambda}(p+q, p) b_{\mu\lambda}(p+q, p+q-q')\,(n_{p\lambda-} - n_{p+q\mu+}),$$

$$h_\lambda(q, q') = \frac{4}{N} \sum_{pp'\mu} [\delta_{\lambda\mu} b^*_{\lambda\lambda}(p+q, p) b_{\lambda\lambda}(p'+q', p')\,(-n_{p+q\lambda+} n_{p'+q\lambda+}$$

$$+n_{p\lambda-}n_{p'+q'\lambda+}-n_{p\lambda-}n_{p'\lambda-}+n_{p+q\lambda+}n_{p'\lambda-})+b^{*}_{\lambda\mu}(p+q,\,p)b_{\lambda\mu}(p+q',\,p)n_{p'\lambda-}(n_{p\mu-}-n_{p+q\lambda+})$$

$$+b^{*}_{\mu\lambda}(p+q,\,p)b_{\mu\lambda}(p+q,\,p+q-q')n_{p'\lambda+}(n_{p+q\mu+}-n_{p\lambda-}). \tag{44}$$

To calculate the magnon energy from the effective Hamiltonian we shall use the Green function method. Let $G_{qq'}(\omega)$ denote the time Fourier transform of the retarded Green function $\langle\langle\beta_q(t);\,\beta^{\dagger}_{q'}\rangle\rangle$. We get the following equation of motion

$$(\omega-E_q)G_{qq'}(\omega)=\delta_{qq'}+\sum_{k\neq q}\varphi_{\alpha\lambda}(q-k)T_{\alpha\lambda}(q,\,k)G_{kq'}(\omega), \tag{45}$$

where

$$E_q=E^0_q+\sum_{\alpha\lambda}\varphi_{\alpha\lambda}(0)T_{\alpha\lambda}(q,\,q).$$

Let us define the function

$$\tilde{\varphi}_{\lambda}(q)=\varphi_{2\lambda}(q)-\langle\varphi_{2\lambda}(q)\rangle, \tag{46}$$

$\langle\ldots\rangle$ denotes configuration average. Observing that $\varphi_{1\lambda}(q)-\langle\varphi_{1\lambda}(q)\rangle=-\tilde{\varphi}_{\lambda}(q)$ and using definition (46) we can rewrite equation (45) in the form

$$(\omega-E_q)G_{qq'}(\omega)=\delta_{qq'}+\sum_{k\alpha\lambda}\tilde{\varphi}_{\lambda}(q-k)\,(-1)^{\alpha}T_{\alpha\lambda}(q,\,k)G_{kq'}(\omega). \tag{47}$$

The magnon energies are determined by poles of the Green function averaged over configurations of atoms $\langle G_{qq'}(\omega)\rangle$. Similarly as in [3] one can observe that for $\lambda\neq\mu$

$$\langle\tilde{\varphi}_{\lambda}(k_1)\ldots\tilde{\varphi}_{\lambda}(k_m)\tilde{\varphi}_{\mu}(k_{m+1})\ldots\varphi_{\mu}(k_n)\rangle$$

$$=\langle\tilde{\varphi}_{\lambda}(k_1)\ldots\tilde{\varphi}_{\lambda}(k_m)\rangle\,\langle\tilde{\varphi}_{\mu}(k_{m+1})\ldots\tilde{\varphi}_{\mu}(k_n)\rangle, \tag{48}$$

due to properties of $c^{\alpha\lambda}_i$.

It is convenient to use the Kaneyoshi iteration-decoupling procedure [7], and express the averages of products of the stochastic functions $\tilde{\varphi}_{\lambda}(q)$ in terms of the cumulant averages [10]. As a result we get the averaged Green function in the form

$$G_{q,q'}(\omega)=\delta_{qq'}[\omega-E_q-\Gamma_q(\omega)]^{-1}. \tag{49}$$

The self-energy part $\Gamma_q(\omega)$ can be written as a sum $\Gamma_q(\omega)=\Gamma^{(1)}_q(\omega)+\Gamma^{(2)}_q(\omega)+\ldots$ of contributions associated with single-site scattering, tones due to effects of pairs of scattering centres etc. The single-site scattering contribution for all orders is given by

$$\Gamma^{(1)}_q(\omega)=\sum_{\lambda}\Bigg[P_2(x_\lambda)\sum_{\alpha_1\alpha_2}(-1)^{\alpha_1+\alpha_2}\frac{4}{N}\sum_{k}T_{\alpha_1\lambda}(q,\,k)G^{(0)}_{k}T_{\alpha_2\lambda}(k,\,q)$$

$$+\ldots P_n(x_\lambda)\sum_{\alpha_1\ldots\alpha_n}(-1)^{\alpha_1+\ldots+\alpha_n}\left(\frac{4}{N}\right)^{n-1}\sum_{k_1\ldots k_{n-1}}T_{\alpha_1\lambda}(q,\,k_1)G^{(0)}_{k_1}T_{\alpha_2\lambda}(k_1k_2)G^{(0)}_{k_2}\ldots$$

$$\ldots T_{\alpha_n\lambda}(k_{n-1},\,q)+\ldots, \tag{50}$$

where $G_k^{(0)} = (\omega - E_k)^{-1}$, $P_n(x_\lambda)$ are the Matsubara–Yonezawa [10] polynomials and $x_1 = 3(1-p)$, $x_2 = x_3 = x_4 = p$.

We can expand $f_\lambda(q, q')$ and $h_\lambda(q, q')$ in the long-wavelengths limit as follows

$$f_\lambda(q, q') = f_\lambda^{(1)} \boldsymbol{q} \cdot \boldsymbol{q}' + f_\lambda^{(2)} q'^2,$$

$$h_\lambda(q, q') = h_\lambda^{(1)} \boldsymbol{q} \cdot \boldsymbol{q}' + h_\lambda^{(2)} q'^2, \tag{51}$$

where

$$f_\lambda^{(1)} = \tfrac{1}{3} d_0^2 \sum_{\mu \neq \lambda} \sum_p [(B_{\lambda\mu}^{(1)}(p))^* B_{\lambda\mu}^{(1)}(p) (n_{p\mu-} - n_{p\lambda+})$$
$$- (B_{\mu\lambda}^{(1)}(p))^* B_{\mu\lambda}^{(1)}(p) (n_{p\lambda-} - n_{p\mu+})] |\nabla z_p|^2 - f_\lambda^{(2)},$$
$$f_\lambda^{(2)} = -d_0^2 [\tfrac{1}{6} \sum_p (B_{\lambda\lambda}^{(0)}(p))^2 (n_{p\lambda-}^{(1)} - n_{p\lambda+}^{(1)}) \nabla^2 z_p$$
$$+ \tfrac{1}{3} \sum_p (B_{\lambda\lambda}^{(0)}(p))^2 (n_{p\lambda-}^{(2)} - n_{p\lambda+}^{(2)}) |\nabla z_p|^2,$$
$$h_\lambda^{(1)} = -n_{\lambda+} f_\lambda^{(2)},$$
$$h_\lambda^{(2)} = -h_\lambda^{(1)} + d_0^2 \sum_p B_{\lambda\lambda}^{(0)}(p) (n_{p\lambda-} - n_{p\lambda+}) [\tfrac{1}{6} \sum_p B_{\lambda\lambda}^{(1)}(p) n_{p\lambda+}^{(1)} \nabla^2 z_p$$
$$+ \tfrac{1}{3} \sum_p B_{\lambda\lambda}^{(2)}(p) n_{p\lambda+}^{(2)} |\nabla z_p|^2], \tag{52}$$

and the definitions of $B_{\lambda\mu}^{(r)}(p)$ are analogous to those introduced in formula (39) i.e.

$$B_{\lambda\mu}^{(0)}(p) = B_{\lambda\mu}(p, p),$$

$$B_{\lambda\mu}^{(1)}(p) = \frac{\partial}{\partial z_{p+q}} B_{\lambda\mu}(p+q, p)|_{q=0},$$

$$B_{\lambda\mu}^{(2)}(p) = \frac{\partial^2}{\partial z_{p+q}^2} B_{\lambda\mu}(p+q, p)|_{q=0},$$

$$B_{\lambda\mu}^{(3)}(p) = \frac{\partial}{\partial (q^2)} B_{\lambda\mu}(p+q, p)|_{q=0}. \tag{53}$$

The quantity d_0 is the q-independent part of the magnon normalization factor d_q and reads

$$d_0 = [\sum_p (B_{11}^{(0)})^2 (n_{p1-} - n_{p1+}) + 3 \sum_p (B_{22}^{(0)})^2 (n_{p2-} - n_{p2+})]^{-1/2}. \tag{54}$$

Putting formula (51) into definition (43), one gets the following long-wavelength expansion of $T_{\alpha\lambda}(q, q')$

$$T_{\alpha\lambda}(q, q') = a_{\alpha\lambda} \boldsymbol{q} \cdot \boldsymbol{q}' + g_{\alpha\lambda} q'^2, \tag{55}$$

where

$$a_{\alpha\lambda} = [t_\alpha - t_\lambda(\omega)] f_\lambda^{(1)} + [I_\alpha - I_\lambda(\omega)] h_\lambda^{(1)},$$
$$g_{\alpha\lambda} = [t_\alpha - t_\lambda(\omega)] f_\lambda^{(2)} + [I_\alpha - I_\lambda(\omega)] h_\lambda^{(2)}. \tag{56}$$

Let us now turn back to the examination of poles of the Green function (49). To get the explicit form of the spin wave stiffness constant the parabolic density of states of unperturbed magnon states up to a certain cut-off value and vanishing density of states for higher energies was assumed and the coefficients $T_{\alpha\lambda}(q, q')$ were taken in form (55). We found the following formula for the spin wave stiffness constant, including both the "average exchange" and the "magnon scattering" terms

$$D(p) = D_0(p) + \sum_{\lambda} \sum_{n=2}^{\infty} P_n(x_\lambda) \left[3 \left(\frac{a_{2\lambda} - a_{1\lambda}}{3} \right)^n + (g_{2\lambda} - g_{1\lambda})^n \right] [D_0(p)]^{1-n}, \tag{57}$$

where

$$D_0(p) = D_{\text{av.exch.}} + \sum_{\lambda} x_\lambda [(a_{2\lambda} - a_{1\lambda}) + (g_{2\lambda} - g_{1\lambda})]. \tag{58}$$

5. *Summary*

A method for calculating the magnon energy in itinerant electron ferromagnetic alloys AB_3 having a non-vanishing long-range order parameter was developed. It was shown that in the CPA equations for the proposed four-sublattice model it is easy to replace the summations over $\boldsymbol{k}$ space by one dimensional integrals thus making the formulas convenient for numerical analysis.

The problem of effect of ordering was formulated in two steps. First unperturbed magnons have been defined but already for the effective medium with potentials determined in CPA. Next the renormalization of magnon energy due to the deviations from effective potentials was calculated by a perturbational procedure. The numerical analysis of the general formula (57) for the magnon energy stiffness constant is under way and will be published elsewhere.

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REFERENCES

[1] K. Mikke, J. Jankowska, Z. Osetek, A. Modrzejewski, *J. Phys.* **F7**, L211 (1977).
[2] F. Menzinger, F. Sacchetti, R. Teichner, *Solid State Commun.* **9**, 1579 (1971).
[3] J. Morkowski, Transition Metals 1977: Inst. Phys. Conf. Ser. No. 39, pp. 548–53 (1978).
[4] J. Morkowski, *Acta Phys. Pol.* **A43**, 809 (1973).
[5] J. Morkowski, *Physica* **86–88B**, 343 (1977).
[6] I. Takahashi, D. M. Edwards, *J. Phys.* **F8**, 2579 (1978).
[7] T. Kaneyoshi, *Prog. Theor. Phys.* **42**, 477 (1969).
[8] B. Velicky, S. Kirkpatrick, H. Ehrenreich, *Phys. Rev.* **175**, 747 (1968).
[9] D. M. Edwards, W-Y P. Fung, *J. Phys.* **F8**, 2183 (1978).
[10] T. Matsubara, F. Yonezawa, *Prog. Theor. Phys.* **34**, 871 (1965); **37**, 1346 (1967).