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EFFECTIVE MAGNON HAMILTONIAN FOR ITINERANT-ELECTRON FERROMAGNETICS: I. OUTLINE OF THE METHOD

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A method of an effective Hamiltonian for magnons in the itinerant-electron ferromagnetics is formulated. The method reveals close analogies between the behaviour of magnons in the itinerant and localized electron ferromagnetics, and is of particular use for a simplified but systematic treatment of magnon interaction. The effective Hamiltonian is derived for the case of strong itinerant ferromagnetism in a single narrow band, and simple applications are described.

1. *Introduction*

In the itinerant electron model of ferromagnetism a magnon is defined as a bound state of an electron and a hole of opposite spin [1]. The spin of the electron from the electron-hole pair is antiparallel to the total spin momentum of the system of itinerant electrons and the electron-hole bound state corresponds to the propagation of a spin reversal, in close analogy with magnon in localized electron ferromagnets.

It is the purpose of the present paper to explore this analogy by introducing an effective Hamiltonian expressed in terms of boson operators for the creation and annihilation of magnons, similar to the well-known boson representation of the Heisenberg exchange Hamiltonian (see, *e. g.*, [2]). The idea of the effective Hamiltonian is based on intuitive arguments; it is simple, but it seems reasonably accurate; it is particularly useful for treating various aspects of magnon interaction.

The theory of the effective Hamiltonian was formulated in [3] and applied to the relaxation by 3-magnon processes of dipolar origin in [4]. A hint to the method can be inferred from an early treatment by Izuyama of corrections to the spontaneous magnetization due to the interaction of magnons [5].

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2. *Outline of the method*

Because of the limited availability of the lecture notes [3] it is useful to recall here some of the arguments and to describe briefly the method of the effective Hamiltonian.

For simplicity, we consider the case of strong ferromagnetism in a single narrow band described by the Hubbard Hamiltonian

$$\mathscr{H} = \sum_{k\sigma} \varepsilon_{k\sigma} a_{k\sigma}^{+} a_{k\sigma} + (I/N) \sum_{kk'q} a_{k+q,+}^{+} a_{k,+} a_{k'-q,-}^{+} a_{k,-} \tag{1}$$

where $a_{k\sigma}^{+}(a_{k\sigma})$ are the creation (annihilation) operators for electrons of spin σ in the Bloch states specified by the momentum $\vec{k}$. Let H denotes the magnetic field applied along the z-axis of the coordinate system; then, $\varepsilon_{k\pm} = \varepsilon_k \pm \mu_B H$, where ε_k is the Bloch energy, μ_B the Bohr magneton, I the intra-atomic Coulomb integral, and N denotes the number of atoms in the crystal.

We assume the ground state of $\mathscr{H}$, Eq. (1) to be one with the spin-down band occupied up to the Fermi energy ε_F and the spin-up band completely empty. Such a "strongly ferromagnetic" state can be the ground state of the Hubbard Hamiltonian, at least for certain values of the ratio of the Coulomb integral I to the band width, and for certain concentrations of itinerant electrons (*cf.*, *e. g.*, [6]).

Let $|\Phi_0\rangle$ denote the ground state. We define an operator β_q^{+} of the form

$$\beta_q^{+} = \sum_k b_{k+q,k} a_{k+q,+}^{+} a_{k,-}. \tag{2}$$

Within the Random Phase Approximation (RPA) the state $\beta_q^{+}|\Phi_0\rangle$ is an eigenstate of the Hamiltonian (1) [1, 7]. Such a state represents a magnon of wave vector $\vec{q}$, and the operator β_q^{+} can be interpreted as the creation operator of a magnon $\vec{q}$. The energy E_q of the state $\beta_q^{+}|\Phi_0\rangle$, or the magnon energy (the ground state energy is taken as zero), is found by solving the equation [1, 7]

$$(I/N) \sum_{\substack{k \\ (\varepsilon_k < \varepsilon_F)}}' (\varepsilon_{k+q} - \varepsilon_k + \Delta - E_q)^{-1} = 1. \tag{3}$$

Here, Δ denotes the splitting energy of the spin-up and spin-down electrons, *i. e.*,

$$\Delta = nI + 2\mu_B H \tag{4}$$

where n is the number of itinerant electrons per atom.

The coefficients $b_{k+q,k}$, as calculated in RPA from the eigenvalue equation $\mathscr{H}\beta_q^{+}|\Phi_0\rangle = E_q \beta_q^{+}|\Phi_0\rangle$, are [1, 7],

$$b_{k+q,k} = \frac{d_q}{\varepsilon_{k+q} - \varepsilon_k + \Delta - E_q}. \tag{5}$$

It is convenient to determine the normalization constant d_q from the condition

$$\sum_{\substack{k \\ (\varepsilon_k < \varepsilon_F)}}' |b_{k+q,k}|^2 = 1, \tag{6}$$

whereupon

$$|d_q| = \{ \sum_{\substack{k \\ (\varepsilon_k < \varepsilon_F)}}' (\varepsilon_{k+q} - \varepsilon_k + \Delta - E_q)^{-2} \}^{-1/2}, \quad (6')$$

with an arbitrary phase factor.

The magnon creation operators β_q^+ and their Hermitian-adjoint magnon annihilation operators β_q satisfy the commutation rules

$$[\beta_q^+, \beta_{q'}^+] = 0 \quad (7a)$$

and, in the Random Phase Approximation,

$$[\beta_q, \beta_{q'}^+]_{\text{RPA}} = \delta_{qq'}. \quad (7b)$$

Condition (6) is imposed in order to have $[\beta_q, \beta_q^+] = 1$ within RPA.

The operators β_q^+ and β_q can be used to develop a formulation of the theory of magnons in itinerant-electron ferromagnetics which is completely analogous to the spin-wave theory of the Heisenberg localized-spin ferromagnetics. Such a formulation is useful since, first of all, it points up some properties of ferromagnets which appear to be model--independent and, second, it enables one to apply some results derived for Heisenberg ferromagnetics to the itinerant-electron model. Some examples of applications of the method will be described in a subsequent paper [8].

3. *Effective Hamiltonian*

Unfortunately, the theory of the effective Hamiltonian cannot be formulated rigorously. It is necessary to use intuitive arguments which, however, have fairly sound physical grounds.

Let us recall what we know about the low-lying excited states of the Hamiltonian (1). The simplest single excitation from the ground state $|\Phi_0\rangle$ are the Stoner electron-hole pair described by the wave function $|\psi_{k+q,k;\sigma}\rangle = a_{k+q,\sigma}^+ a_{k,-}|\Phi_0\rangle$. Here $\vec{k}$ is restricted by the condition $\varepsilon_k < \varepsilon_F$ and, for $\sigma = -$, $\vec{q}$ should satisfy the condition $\varepsilon_{k+q} > \varepsilon_F$. In the Hartree-Fock approximation $|\psi_{k+q,k;\sigma}\rangle$ are the eigenstates of the Hamiltonian (1) with excitation energies equal to $\mathscr{E}_q^{--} = \varepsilon_{k+q} - \varepsilon_k$ or $\mathscr{E}_q^{+-} = \Delta + \varepsilon_{k+q} - \varepsilon_k$ for $\sigma = -$ or $+$, *i.e.*, for Stoner pairs with and without spin reversal, respectively. The energy needed to reverse the spin of the spin-down electron without changing its Bloch energy is relatively high (typically it is of the order of magnitude of a few tenths of one electronvolt). For excited states with sufficiently small momentum q the interactions between electrons which are neglected in the Hartree-Fock approximation favour the electron-hole bound state energetically.

For small enough momentum q of the excited state, the free Stoner pair with spin reversal, $|\psi_{k+q,k;+}\rangle$, has a much higher energy than the corresponding bound state or magnon. Thus the low-lying energy levels of an itinerant electron ferromagnet are determined by small-q, free Stoner pairs without spin reversal, and by magnons of small q. On the other hand, the population of small-q Stoner pairs with spin reversal can be assumed to be negligible because of their relatively high energy. Stoner pairs without spin reversal are of little relevance to magnetic properties as such. They influence the temperature dependence of thermodynamic quantities and they can be taken into account separately. Here we will be interested in magnons and we shall extract from the full Hamiltonian, (1), those parts which approximately correspond to the energy of the system of magnons in the itinerant-electron system. This will be what we shall call the effective magnon Hamiltonian. The remainder will correspond to the total energy of Stoner pairs without spin reversal and, with our system having $|\Phi_0\rangle$ as its ground state, we will be able to approximate this term by an expression like $\mathscr{H}_{\text{Stoner pair}} = \sum_k \varepsilon_{k-} a_{k-}^+ a_{k-}$ (no electron-hole pairs of spin + are possible for our ground state $|\Phi_0\rangle$).

The effective Hamiltonian will be formally constructed as an expansion in products of the magnon creation and annihilation operators β_q^+, β_q. The obvious requirements of hermiticity and of conservation of the crystal momentum can be used to restrict possible choices of products of the operators β_q^+, β_q entering into the effective Hamiltonian. Further simplifications follow if, for instance, we can presume, as is indeed the case for the system described by the Hamiltonian (1), that the effective Hamiltonian should conserve the total number of magnons. It should be pointed out that actually there is no ambiguity in the final effective Hamiltonian: had we not made explicit use of the above general properties, the spurious terms in the effective Hamiltonian would have ultimately vanished.

The Hubbard Hamiltonian (1) commutes with the total magnetic moment of the system of itinerant electrons, $-\mu_B \Sigma_{k\sigma} \sigma a_{k\sigma}^+ a_{k\sigma}$. Therefore we expect that the corresponding effective Hamiltonian will conserve the total number of magnons (which is proportional to the total magnetic moment). The most general form of the effective Hamiltonian, up to terms of fourth order, and apart from a trivial constant, will be

$$\mathscr{H}_e = \sum_q K_q \beta_q^+ \beta_q + \sum_{kk'q} \Gamma_{kk'}^q \beta_{k+q}^+ \beta_{k'-q}^+ \beta_k \beta_{k'}. \tag{8}$$

Higher order terms can be included, if necessary, for particular cases. The coefficients K_q, $\Gamma_{kk'}^q$ *etc.* can be formally written as follows:

$$K_q = [\beta_q, [\mathscr{H}_e, \beta_q^+]], \tag{9a}$$

$$\Gamma_{kk'}^q = \tfrac{1}{4}[\beta_{k+q}, [\beta_{k'-q}, [[\mathscr{H}_e, \beta_{k'}^+], \beta_k^+]]]. \tag{9b}$$

We use the relations (9) to define the coefficients of the effective magnon Hamiltonian $\mathscr{H}_e$ which is equivalent to the Hamiltonian of a system of itinerant electrons, $\mathscr{H}$:

$$K_q = \langle\Phi_0| [\beta_q, [\mathscr{H}, \beta_q^+]] |\Phi_0\rangle, \tag{10a}$$

$$\Gamma_{kk'}^q = \tfrac{1}{4}\langle\Phi_0| [\beta_{k+q}, [\beta_{k'-q}, [[\mathscr{H}, \beta_{k'}^+], \beta_k^+]]] |\Phi_0\rangle. \tag{10b}$$

The averages are taken with respect to the ground state $|\Phi_0\rangle$.

We express the magnon operators β_q^+, β_q in terms of the electron operators $a_{k\sigma}^+$, $a_{k\sigma}$ through Eq. (2) together with Eqs (3)–(6). The coefficients (10) of the effective Hamiltonian can then be determined by simple, if rather tedious, calculations. For K_q we obtain

$$K_q = \sum_k (\varepsilon_{k+q} - \varepsilon_k + \Delta) |b_{k+q,k}|^2 n_k - (N/I) d_q^2, \tag{11}$$

where $n_k = \langle \Phi_0 | a_{k-}^{+} a_{k-} | \Phi_0 \rangle$ is the ground state occupation number for electrons of spin $-$; n_k equals 1 for $\varepsilon_k < \varepsilon_F$ and is zero otherwise. Using Eqs (5) and (6) we obtain the simple result $K_q = E_q$, E_q being the magnon energy determined by Eq. (3), as it should be for consistency.

The second term in the effective Hamiltonian (8) describes two-body interaction between magnons. $\Gamma_{kk'}^{q}$ is given by

$$\Gamma_{kk'}^{q} = \tfrac{1}{4}(\overline{\Gamma}_{kk'}^{q} + \overline{\Gamma}_{k'k}^{-q} + \overline{\Gamma}_{kk'}^{k'-k-q} + \overline{\Gamma}_{k'k}^{-k'+k+q}), \tag{12a}$$

$$\begin{aligned}\overline{\Gamma}_{kk'}^{q} = &-(I/N) \sum_{pp'} b_{p+k',p} b_{p'+k+q,p'+q} b^{*}_{p+k'-q,p} b^{*}_{p'+k+q,p'} n_p n_{p'} + \\ &+(I/N) \sum_{pp'} b_{p+k',p} b_{p+k+q,p+q} b^{*}_{p'+k'-q,p'} b^{*}_{p+k+q,p} n_{p'} n_{p},\end{aligned} \tag{12b}$$

(see [8]).

An expression of the form (10b) was used by Izuyama [5] to study the effect of magnon interaction on thermodynamic properties of itinerant ferromagnetics.

4. *Generalizations*

No essentially new results have been reported so far, except for a formulation of a systematic approach to magnons and their interaction in itinerant ferromagnetics, which is easy to generalize for more complicated cases as, for instance, for several bands or Hamiltonians with relativistic effects included.

As an example of such a generalization we shall consider the system of itinerant electrons in a single narrow band, taking into account the magnetic dipolar interactions between electrons. The total Hamiltonian of the system will consist of the Hubbard Hamiltonian (Eq. (1)), plus the energy of the dipolar interactions. The dipolar part of the Hamiltonian for the multi-band case was given in [9]. We can use this result, suppressing band indices in Eq. (12) of [9]. The total Hamiltonian will now be given by

$$\begin{aligned}\mathscr{H} = &\sum_{k\sigma} \varepsilon_{k\sigma} a_{k\sigma}^{+} a_{k\sigma} + (I/N) \sum_{kk'q} a_{k+q,+}^{+} a_{k,+} a_{k'-q,-}^{+} a_{k',-} - \\ &- N^{-1} \sum_{kk'q} \{ D_q (a_{k+q,+}^{+} a_{k,+} a_{k'-q,-}^{+} a_{k',-} + \\ &+ a_{k+q,+}^{+} a_{k,-} a_{k'-q,-}^{+} a_{k',+} - \tfrac{1}{2} a_{k+q,+}^{+} a_{k,+} a_{k'-q,+}^{+} a_{k',+} - \\ &- \tfrac{1}{2} a_{k+q,-}^{+} a_{k,-} a_{k'-q,-}^{+} a_{k',-}) + \\ &+ [A_q a_{k+q,+}^{+} a_{k,-} (a_{k'-q,+}^{+} a_{k',+} - a_{k'-q,-}^{+} a_{k',-}) + \\ &+ B_q a_{k+q,+}^{+} a_{k,-} a_{k'-q,+}^{+} a_{k',-} \qquad + \text{h.c.}] \}.\end{aligned} \tag{13}$$

The coefficients are defined as follows

$$D_q = (2\mu_B^2 N/V)\, |F(\vec{q})|^2 \int d\vec{r} r^{-3} [1 - 3(z/r)^2] e^{-i\vec{q}\cdot\vec{r}}, \tag{14a}$$

$$A_q = (3\mu_B^2 N/V)\, |F(\vec{q})|^2 \int d\vec{r} r^{-5} (x - iy) z e^{-i\vec{q}\cdot\vec{r}}, \tag{14b}$$

$$B_q = (\tfrac{3}{2}\mu_B^2 N/V)\, |F(\vec{q})|^2 \int d\vec{r} r^{-5} (x - iy)^2 e^{-i\vec{q}\cdot\vec{r}}. \tag{14c}$$

Integration in Eqs (14) extends over the volume V of the crystal. $F(\vec{q})$ is the magnetic form-factor, defined in terms of the Wannier function $\varphi(\vec{r})$ of itinerant electrons as follows:

$$F(\vec{q}) = \int d\vec{r}|\varphi(\vec{r})|^2 e^{i\vec{q}\cdot\vec{r}}. \tag{14d}$$

In practical calculations we shall be interested in the coefficients A_q, B_q, D_q for small q (that is, q small as compared with the inverse lattice constant but larger than the inverse of the linear dimension of the ferromagnetic sample). For this long-wavelengths limit we have

$$A_q = Dq_z q_+/q^2, \tag{15a}$$

$$B_q = -\tfrac{1}{2}D(q_-/q)^2. \tag{15b}$$

$$D_q = 2D[(q_z/q)^2 - \tfrac{1}{3}], \tag{15c}$$

where

$$D = 4\pi\mu_B^2 N/V, \tag{15d}$$

and $q_\pm = q_x \pm iq_y$. In the long-wavelengths limit the magnetic form-factor has been replaced by unity (*cf.* [4], there are two misprints in formula (2) of [4]: B_q should be replaced by $-B_q$ and the right-hand side of the expression for D_q should be multiplied by the factor 2).

For $q = 0$ the arguments leading to Eqs (15) cannot be used. Instead, for a sample in the form of an ellipsoid of revolution we have

$$D_0 = D(N_z - \tfrac{1}{3}), \tag{15e}$$

where N_z is the demagnetizing factor for the symmetry axis (taken parallel to the applied magnetic field). A_0 and B_0 vanish in this case.

The Hamiltonian (13) does not conserve the total magnetic moment; therefore, in constructing the effective Hamiltonian equivalent to (13) it is not admissible to restrict oneself solely to terms conserving the number of magnons. The general form of the effective Hamiltonian up to terms of fourth order in the magnon operators is

$$\begin{aligned}\mathscr{H}_e = &\sum_q \{K_q\beta_q^+\beta_q + (L_q\beta_q\beta_{-q} + \text{h.c.})\} + \\ &+ \sum_{qq'} (C_{qq'}\beta_{q+q'}^+\beta_q\beta_{q'} + \text{h.c.}) + \\ &+ \sum_{kk'q} G_{kk'}^q \beta_{k+q}^+\beta_{k'-q}^+\beta_k\beta_{k'} + \\ &+ \sum_{qq'q''} (F_{qq'q''}\beta_{q+q'+q''}^+\beta_q\beta_{q'}\beta_{q''} + \text{h.c.}).\end{aligned} \tag{16}$$

K_q and $G_{kk'}^q$ are given by the right-hand sides of Eqs (10a) and (10b), respectively, for the Hamiltonian (13), and

$$L_q = \tfrac{1}{2}\langle\Phi_0|\,[[\mathscr{H}, \beta_q^+], \beta_{-q}^+]\,|\Phi_0\rangle, \tag{17a}$$

$$C_{qq'} = \tfrac{1}{2}\langle\Phi_0|\,[\beta_{q+q'}, [[\mathscr{H}, \beta_q^+], \beta_{q'}^+]]\,|\Phi_0\rangle, \tag{17b}$$

$$F_{qq'q''} = \tfrac{1}{6}\langle\Phi_0|\,[\beta_{q+q'+q''}, [[[\mathscr{H}, \beta_{q''}^+], \beta_{q'}^+], \beta_q^+]]\,|\Phi_0\rangle. \tag{17c}$$

Strictly speaking, terms proportional to $\beta_q\beta_{q'}\beta_{-q-q'}$ and similar higher-order terms could also appear in the effective Hamiltonian (16). We shall neglect such terms since, in the first approximation at least, they do not contribute either to magnon energies or to the magnon relaxation rates.

4. *Applications*

The simplest example of application of the effective Hamiltonian is the calculation of corrections to the magnon energy coming from dipolar interactions of the itinerant electrons. In the first approximation the effective Hamiltonian is restricted to the second order terms of the right-hand side of Eq. (16). From (10a), (17a) and (13) we obtain

$$K_q = E_q - N|d_q/I|^2 D_q - 2D_0 + \\ + N^{-1}\sum_{kq'} D_{q'}\{b_{k+q,k}b^*_{k+q+q',k+q'}n_k n_{k+q'} + \\ + |b_{k+q,k}|^2 n_k n_{k+q+q'} + \tfrac{1}{2}|b_{k+q,k}|^2 n_k n_{k+q'}\}, \tag{18}$$

and

$$L_q = N|d_q/I|^2 B^*_q + \\ + N^{-1}\sum_{kq'} B^*_{q'} b_{k-q',k-q'-q} b_{k-q,k}\{n_k + n_{k-q-q'} - 2n_k n_{k-q-q'}\}. \tag{19}$$

The second-order part of the effective Hamiltonian can be diagonalized by the well--known Holstein-Primakoff transformation [10]. The magnon energy corrected by dipolar contribution is now given by

$$\tilde{E}_q = \{K_q^2 - |2L_q|^2\}^{1/2}. \tag{20}$$

The uncorrected magnon energy E_q is determined by condition (3), which is valid within RPA. For long-wavelength magnons the solution of Eq. (3) is of the following general form:

$$E_q = 2\mu_B H + \alpha q^2. \tag{21}$$

The magnon energy coefficient α depends on details of the band structure and the Fermi surface. The Random Phase Approximation is actually too crude to be used for calculating α quantitatively, even for known band structures. Considerable efforts have been made to calculate the coefficient α accurately, taking into account many-body effects beyond RPA, (see, for instance, [11]), and for the real band structure [12].

Dipolar corrections are significant only in the limit of long magnon wavelength. In this limit it is justifiable to neglect those parts of the dipolar corrections which are proportional to q^2 (and, obviously, all higher powers of q) since they are by a few orders of magnitude smaller than the corresponding exchange term αq^2. Then we obtain

$$K_q \cong E_q - 2D_0 + D_q + O(Dq^2), \tag{22a}$$

$$L_q = B^*_q + O(Dq^2). \tag{22b}$$

From Eqs (20)–(22) it follows that

$$E_q = \{[2\mu_B(H-4\pi MN_z)+\alpha q^2]\,[2\mu_B(H-4\pi MN_z)+ +\alpha q^2+8\pi M\mu_B \sin^2 \Theta_q]\}^{1/2}, \tag{23}$$

with M standing for saturation magnetization, $M = nN\mu_B/V$ and Θ_q being the angle between the magnon wave vector $\vec{q}$ and the magnetic field direction which is parallel to the z-axis. A more accurate calculation, taking into account terms proportional to Dq^2, (which are neglected in Eqs (22)) leads to the same expression as in Eq. (23) but with the coefficient α slightly modified by the magnetic field H and the dipolar terms, *cf.* [9]. $\tilde{E}_q$ of Eq. (23) is equivalent to the standard expression for the long-wavelength magnon energy with dipolar corrections for localized spin ferromagnetics, derived by Holstein and Primakoff [10]. Thus the form of the dispersion relation for long-wavelength magnons appears to be the same for the two extreme cases of localized or itinerant magnetic electrons. This observation encourages one to seek other properties which are essentially model-independent. It appears that the effective magnon Hamiltonian itself may be considered as in a sense model-independent. For instance, magnon relaxation rates in the first approximation are the same for both models, allowing for the obvious difference in the exchange parameters. An example of the application of the effective Hamiltonian to the calculation of magnon relaxation rates had been described earlier [4], another case is being considered in the next paper.

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