

# A new approach to the RKKY interaction

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## Abstract

We propose a new method for the RKKY interaction, in which an expression derived by Nolting *et al.* (1997) is combined with the single-site approximation for the  $s$ - $f$  model by Takahashi *et al.* (1996)

## 1 Introduction

Indirect localized-spin exchange-interaction via conduction electrons is known as the RKKY interaction [1, 2, 3]. The "original" expression for the RKKY interaction was derived by using the second order perturbation in the exchange interaction between a conduction electron and localized spins. Therefore, the "original" RKKY interaction is valid for a system having weak exchange interaction and/or broad conduction band. Recently, Nolting *et al.* [4, 5] derived an improved RKKY interaction expression considering the higher order effect of exchange interaction.

In this brief note, we follow the work by Nolting *et al.* with using Green's function which is familiar to us. The physical meaning of the assumption made by Nolting *et al.* is discussed in detail. In addition, we propose a new calculation method for the RKKY interaction, in which the single-site approximation is used in order to describe the conduction electron state. [6]

Our final goal is to understand the relation between the magnetic order of the local magnetic moment and the itinerant electrons states. In the discussion we mention the problem we should grapple with for the above purpose.

## 2 Basic Consideration

### 2.1 $s$ - $f$ Model and Green's function

The  $s$ - $f$  model describes the exchange coupling of itinerant electrons ( $s$  electron) to localized magnetic moments ( $f$  spins). The Hamiltonian is given by

$$H = H_s + H_{sf} , \quad (1)$$

with

$$H_s = \sum_{k,\mu} \varepsilon_k a_{k,\mu}^\dagger a_{k,\mu} = \sum_{m,n,\mu} \varepsilon_{m,n} a_{m,\mu}^\dagger a_{n,\mu} , \quad (2)$$

$$H_{sf} = -I \sum_{m, \nu, \mu} (\sigma_{\nu\mu} \cdot S_m) a_{m\nu}^\dagger a_{m\mu} = -\frac{I}{N} \sum_m \sum_{k, q, \nu, \mu} e^{iq \cdot m} (\sigma_{\nu\mu} \cdot S_m) a_{k+q\nu}^\dagger a_{k\mu} . \quad (3)$$

The meaning of notation is the same as we have used until now.

We define the Green's function  $G$  and unperturbed Green's function  $G_0$  by

$$G \equiv G(E) = \frac{1}{E - H} = \frac{1}{E - H_s - H_{sf}} , \quad (4)$$

$$G_0 \equiv G_0(E) = \frac{1}{E - H_s} . \quad (5)$$

Thus, (see Eqs. (4.4) and (4.5) in Ref [5])

$$G = G_0 + GH_{sf}G_0 , \quad (6)$$

$$G = G_0 + G_0H_{sf}G . \quad (7)$$

It should be noted that  $GH_{sf} \neq H_{sf}G$  because both  $H_{sf}$  and  $G$  include  $f$  spin operator. On the other hand,  $G_0G = GG_0$  and  $G_0H_{sf} = H_{sf}G_0$  because  $G_0$  includes no  $f$  spin operator. Both Eqs. (6) and (7) are still exact. However, when we use any approximation for spin operators, it cannot avoid to introduce the error that arises from the noncommutation. In order to decrease (or compensate) the error, we use the following relation combining the above equations (see Eq.(4.7) in Ref. [5]);

$$G = G_0 + \frac{1}{2}[GH_{sf}G_0 + G_0H_{sf}G] . \quad (8)$$

## 2.2 Modified RKKY interaction

We consider the indirect  $f$  spin coupling mediated by the spin-polarized band-electrons through the  $s$ - $f$  exchange interaction. In order to transform  $H_{sf}$  into an "effective" spin Hamiltonian  $H_f$ , we need to average  $H_{sf}$  in the subspace of the conduction electrons;

$$H_f = -I \sum_m \sum_{q, \mu, \nu} e^{iq \cdot m} (\sigma_{\nu\mu} \cdot S_m) \frac{1}{N} \sum_k < a_{k+q\nu}^\dagger a_{k\mu} >^{(s)} . \quad (9)$$

In Eq. (9),  $< a_{k+q\nu}^\dagger a_{k\mu} >^{(s)}$  represents the effect of the operator  $a_{k+q\nu}^\dagger a_{k\mu}$  acting on  $f$  spins under the situation considered. Note the condition that the electronic system described by the Hamiltonian  $H$  has a energy  $E$  is given by

$$\delta(E - H) = -\frac{1}{\pi} \text{Im} G(E) \left( = -\frac{1}{\pi} \text{Im} \frac{1}{E - H} \right) . \quad (10)$$

Thus,  $< a_{k+q\nu}^\dagger a_{k\mu} >^{(s)}$  can be defined by

$$< a_{k+q, \nu}^\dagger a_{k, \mu} >^{(s)} \equiv \int_{-\infty}^{+\infty} dE f_-(E) < 0 | a_{k, \mu} \delta(E - H) a_{k+q, \nu}^\dagger | 0 > , \quad (11)$$

$$= \int_{-\infty}^{+\infty} dE f_-(E) < k, \mu | \delta(E - H) | k + q, \nu > , \quad (12)$$

$$= -\frac{1}{\pi} \int_{-\infty}^{+\infty} dE f_-(E) < k, \mu | \text{Im} G(E) | k + q, \nu > , \quad (13)$$

where  $f_-(E)$  is the Fermi function. It is worth noting that the non-diagonal term of  $< a_{k+q, \nu}^\dagger a_{k, \mu} >^{(s)}$  corresponds to non-uniform distribution of electrons (see later discussion).

Most important problem we should discuss hereafter is how to calculate reasonable  $\langle k, \mu | \text{Im} G(E) | k + q, \nu \rangle$ . For the expression of  $G$  given by Eq. (8), we have the following matrix element:

$$\begin{aligned} \langle k, \mu | G(E) | k + q, \nu \rangle &= G_0(k, E) \delta_{q,0} \delta_{\mu,\nu} \\ &+ \frac{1}{2} \left[ \sum_{k', \sigma} \langle k, \mu | G(E) | k', \sigma \rangle \langle k', \sigma | H_{sf} | k + q, \nu \rangle G_0(k + q, E) \right. \\ &\left. + \sum_{k', \sigma} G_0(k, E) \langle k, \mu | H_{sf} | k', \sigma \rangle \langle k', \sigma | G(E) | k + q, \nu \rangle \right], \end{aligned} \quad (14)$$

where  $G_0(k) \equiv G_0(k, E) \equiv \langle k, \mu | G_0(E) | k, \mu \rangle$  (independent of spin index  $\mu$ ). It should be insisted that Equation (14) is still exact. The physical meaning of Eq. (14) is district; The first term of the right-hand side stands for a unperturbed propagator, thus it shows no spin-polarized effect. All effect of spin-polarized electron is represented in the second terms. The spin-polarization of conduction electrons is caused by the  $s$ - $f$  exchange interaction or  $H_{sf}$ . It should be noted that the way up to (from)  $H_{sf}$  is presented by unperturbed propagator  $G_0$ , while the other way from (up to)  $H_{sf}$  is presented by perturbed propagator  $G$ . Note that  $G$  still has a spin-nondiagonal term; this means that the spin-flip process of  $s$  electron may occur on the way up to (from) the  $f$  spin involved in  $H_{sf}$ .

To proceed the calculation, we replace the Green's functions  $G$  on the right-hand-side of Eq. (14) by the  $G_{av}$  which is calculated by the single-site approximation;

$$\langle k, \mu | G(E) | k', \sigma \rangle \rightarrow G_{av}^{\mu}(k, E) \delta_{k,k'} \delta_{\mu,\sigma}, \quad (15)$$

$$\langle k', \sigma | G(E) | k + q, \nu \rangle \rightarrow G_{av}^{\nu}(k + q, E) \delta_{k+q,k'} \delta_{\nu,\sigma}. \quad (16)$$

Note that  $G_{av}$  has no more the spin-flip process.

Then, (see Eq.(4.11) in Ref. [5]);

$$\begin{aligned} \langle k, \mu | G(E) | k + q, \nu \rangle &= G_0(k, E) \delta_{q,0} \delta_{\mu,\nu} \\ &+ \frac{1}{2} [G_{av}^{\mu}(k, E) \langle k, \mu | H_{sf} | k + q, \nu \rangle G_0(k + q, E) \\ &+ G_0(k, E) \langle k, \mu | H_{sf} | k + q, \nu \rangle G_{av}^{\nu}(k + q, E)], \end{aligned} \quad (17)$$

$$\begin{aligned} &= G_0(k, E) \delta_{q,0} \delta_{\mu,\nu} \\ &+ \frac{1}{2} \langle k, \mu | H_{sf} | k + q, \nu \rangle \\ &\quad \times [G_{av}^{\mu}(k, E) G_0(k + q, E) + G_0(k, E) G_{av}^{\nu}(k + q, E)], \end{aligned} \quad (18)$$

$$= G_0(k, E) \delta_{q,0} \delta_{\mu,\nu} + \frac{1}{2} \langle k, \mu | H_{sf} | k + q, \nu \rangle A_{k,\mu}^{k+q,\nu}(E), \quad (19)$$

$$= G_0(k, E) \delta_{q,0} \delta_{\mu,\nu} - \frac{I}{2N} \sum_n e^{-iq \cdot n} (\sigma_{\mu\nu} \cdot S_n) A_{k,\mu}^{k+q,\nu}(E), \quad (20)$$

where, (see Eq.(4.10) in Ref. [5]);

$$A_{k,\mu}^{k+q,\nu}(E) \equiv G_{av}^{\mu}(k, E) G_0(k + q, E) + G_0(k, E) G_{av}^{\nu}(k + q, E), \quad (21)$$

$$\langle k, \mu | H_{sf} | k + q, \nu \rangle = -\frac{I}{N} \sum_m e^{-iq \cdot m} (\sigma_{\mu\nu} \cdot S_m). \quad (22)$$

For the effective spin Hamiltonian Eq. (9), we need the expectation value of  $\frac{1}{N} \sum_k \langle a_{k,\mu}^{\dagger} a_{k+q,\nu} \rangle^{(s)}$  (see Eq.(4.12) in Ref. [5]);

$$\frac{1}{N} \sum_k \langle a_{k,\mu}^{\dagger} a_{k+q,\nu} \rangle^{(s)} = -\frac{1}{\pi N} \text{Im} \int_{-\infty}^{+\infty} dE f_{-}(E) \sum_k G_0(k, E) \delta_{q,0} \delta_{\mu,\nu}$$

$$-\frac{I}{2N} \sum_n e^{-iq \cdot n} (\sigma_{\mu, \nu} \cdot S_n) \left\{ -\frac{1}{\pi N} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) \sum_k A_{k, \mu}^{k+q, \nu}(E) \right\}, \quad (23)$$

$$= \frac{1}{2} \delta_{q,0} \delta_{\mu, \nu} < n > - \frac{I}{2N} \sum_n e^{-iq \cdot n} (\sigma_{\mu, \nu} \cdot S_n) D_q^{\mu, \nu}, \quad (24)$$

where (see Eq.(4.13) in Ref. [5])

$$D_q^{\mu, \nu} \equiv -\frac{1}{\pi N} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) \sum_k A_{k, \mu}^{k+q, \nu}(E), \quad (25)$$

$$= -\frac{1}{\pi N} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) \sum_k [G_{\text{av}}^{\mu}(k, E) G_0(k+q, E) + G_0(k, E) G_{\text{av}}^{\nu}(k+q, E)]. \quad (26)$$

Note  $D_q^{\uparrow\uparrow} + D_q^{\downarrow\downarrow} = D_q^{\uparrow\downarrow} + D_q^{\downarrow\uparrow}$ , and  $D_{\uparrow\downarrow} = D_{\downarrow\uparrow}$ . Inserting Eq. (24) into Eq. (9), we obtain effective  $f$  spin Hamiltonian;

$$H_f = -I \sum_m \sum_{q, \nu, \mu} e^{iq \cdot m} (\sigma_{\nu \mu} \cdot S_m) \frac{1}{N} \sum_k < a_{k+q, \nu}^{\dagger} a_{k, \mu} >^{(s)}, \quad (27)$$

$$= -I \sum_m \sum_{q, \nu, \mu} e^{iq \cdot m} (\sigma_{\nu \mu} \cdot S_m) \left\{ \frac{1}{2} \delta_{q,0} \delta_{\mu, \nu} < n > - \frac{I}{2N} \sum_n e^{-iq \cdot n} (\sigma_{\mu, \nu} \cdot S_n) D_q^{\mu, \nu} \right\}, \quad (28)$$

$$= -\frac{I^2}{2N} \sum_{m, n} e^{iq \cdot (m-n)} \times [S_m^z S_n^z (D_q^{\uparrow\uparrow} + D_q^{\downarrow\downarrow}) (S_m^x S_n^x + S_m^y S_n^y) (D_q^{\uparrow\downarrow} + D_q^{\downarrow\uparrow}) + i(S_m^x S_n^y + S_m^y S_n^x) (D_q^{\uparrow\downarrow} - D_q^{\downarrow\uparrow})], \quad (29)$$

$$= +\frac{I^2}{2N} \sum_{m, n, q} e^{iq \cdot (m-n)} (S_m^x S_n^x + S_m^y S_n^y + S_m^z S_n^z) (D_q^{\uparrow\uparrow} + D_q^{\downarrow\downarrow}), \quad (30)$$

$$= -\sum_{m, n} J_{m, n} S_m \cdot S_n. \quad (31)$$

with

$$J_{m, n} = -\frac{I^2}{2N} \sum_q e^{iq \cdot (m-n)} (D_q^{\uparrow\uparrow} + D_q^{\downarrow\downarrow}). \quad (32)$$

### 3 Discussion and Summary

The 'normal' RKKY interaction is derived using the second order perturbation in the  $s$ - $f$  exchange interaction. Therefore, the expression for the 'normal' RKKY interaction is applicable for the case of weak exchange interaction compared with conduction bandwidth. To improve the RKKY theory, the most important quantity to study is, of course,  $\frac{1}{N} \sum_k < a_{k, \mu}^{\dagger} a_{k+q, \nu} >^{(s)}$ . It should be emphasized that  $< a_{k, \mu}^{\dagger} a_{k+q, \nu} >^{(s)} = \delta_{q,0} \delta_{\mu, \nu}$  when  $G_{\text{av}}$  is used in Eq. (13) instead of original  $G$ . Hence, to take into account of the non-diagonal element of  $G$ , Nolting *et al.* first expand  $G$  up to the first order of  $H_{sf}$  then approximate  $G$  by  $G_{\text{av}}$  in the expansion terms (see Eqs. (8)). In our approach, the multiple scattering is considered by using the averaged Green's function  $G_{\text{av}}$ . Therefore, our approach may extend the application range toward the strong exchange interaction; However, we have not been able to clarify the application range. In addition, we need to investigate the connection between the present theory and double exchange interaction; the double-exchange effect becomes significant when the exchange interaction is strong.

Incorporating the correlation effect between different  $f$  spins brings short-ranged order to  $f$  spins system. Further, it brings the  $k$  dependence in the self-energy of a conduction electron [7, 8]. Thus, incorporating the correlation effect between different  $f$  spins makes the problem rather difficult. Therefore, at first stage, maybe we should proceed within the single-site theory (or mean field theory) both for conduction electrons and for the localized spins. Even in this approach, it should be emphasized that the nondiagonal matrix

element of  $G$  in  $k$  representation is not zero as a consequence of (partly) incorporating the correlation effect (see Eqs. (14) and (20)).

Recently, the carrier-induced ferromagnetism has been reported in the diluted magnetic semiconductors (DMS) as (Ga, Mn)As [9]. The present theory may be applicable for the study of mechanism of ferromagnetism in DMS because of wide-applicability range (or flexibility) for the electron number  $n$  and exchange interaction strength  $IS$ .

Throughout our work, we have neglected the Coulomb interaction between  $s$  electrons. When the conduction band is broad, the Coulomb interaction should be taken into using the form of  $e^2/\epsilon_0 r$  together with the screening effect. On the other hand, when the band is narrow, the Hubbard type Coulomb interaction should be considered because double occupation at one site is significant. Although the problem is difficult, we have no way except to proceed step by step.

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