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Effective indirect multi-site spin–spin interactions in the s–d(f) model

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ABSTRACT

Using the diagram technique for Matsubara Green's functions it is shown that the dynamics of the localized spin subsystem in the s–d(f) model can be described in terms of an effective spin model with multi-site spin–spin interactions. An exact representation of the action for the effective purely spin model is derived as an infinite series in powers of s–d(f) exchange interaction J. The indirect interactions of the 2nd, 3rd and 4th order are discussed.

1. Introduction

Kondo lattice model or s–d(f) exchange model is widely used to describe the correlation effects in metals (and their compounds) with unfilled *d*- and *f*-shells.

The nature of the ground state in these systems is largely determined by the result of competition between two interactions. On the one hand, s–d(f) exchange coupling between spins of itinerant s- and localized d(f)-electrons due to Kondo fluctuations screens the localized spins and tends to form a non-magnetic ground state [1]. In the opposite direction acts indirect exchange (RKKY) interaction between spins of d(f)-electrons [2], trying to set a long-rang magnetic order which is not necessarily a ferromagnetic or antiferromagnetic. Correlation effects can lead to, for example, helical magnetic structures [3], with period that is determined by the Fermi surface singularities [4,5].

It is clear that the study of competition between different effective interactions, that occur in the localized spin subsystem and are caused by the same itinerant electrons, must be carried out within the same unified approach.

The purpose of this paper is to derive such an effective Hamiltonian (or rather action), which will allow to study the localized spin subsystem in the s–d(f) model within the model with only spin–spin interactions.

This problem is solved by integrating charge degrees of freedom using the diagram technique for Matsubara Green's functions. It is shown that in addition to the two-spin indirect exchange interaction, which occurs in the second order in s–d(f)-exchange parameter J, in the following orders also appear terms describing, in particular, the ring and biquadratic exchange interactions. The essential point of all these interactions is the account for retardation effects provided by the imaginary time dependence of all the effective multi-site exchange parameters.

2. The Hamiltonian of the s-d(f) exchange model

The Hamiltonian of the Kondo lattice model (or s–d(f) exchange model) can be written as a sum of two terms:

$$\widehat{H} = \widehat{H}_0 + \widehat{H}_{int}, \tag{1}$$

where

$$\widehat{H}_0 = \sum_{k\alpha} (\varepsilon_k - \mu) c^+_{k\alpha} c_{k\alpha}, \quad \widehat{H}_{int} = \frac{J}{2} \sum_f c^+_f \widetilde{S}_f c_f. \tag{2}$$

Operator $\widehat{H}_0$ stands for the energy of noninteracting current carriers (electrons or holes) with dispersion ε_k, μ the chemical potential. Operator $c^+_{k\alpha}(c_{k\alpha})$ creates (annihilates) a particle in the state with quasimomentum k and spin projection $\alpha = \pm 1/2$.

The second term in (1) describes Kondo exchange interaction between localized spins and itinerant quasiparticles. The intensity of this interaction is defined by the constant J. Operator $\widetilde{S}_f = \overrightarrow{S_f}\overrightarrow{\sigma}$ is a product of a localized spin operator $\overrightarrow{S_f}$ and a vector $\overrightarrow{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ which is formed of Pauli matrices. In definition (2) the spinor notations, $c^+_f = (c^+_{f\uparrow}, c^+_{f\downarrow})$, are used. The operators c_f and c_k are related to each other by Fourier transformation: $c_f = N^{-1/2} \sum_k e^{ikf} c_k$.

3. Spin Green's functions and effective action

The derivation of multi-site spin–spin interactions in the arbitrary order in the coupling constant J is based on integrating the charge

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degrees of freedom using the diagram technique for Matsubara Green's functions [6]:

$$-\langle T_\tau \overline{S}_f^j(\tau)\overline{S}_{f'}^{j'}(\tau')\rangle, \quad j, j' = \{x, y, z\}. \tag{3}$$

In this expression the spin operators are written down in the Heisenberg representation: $\overline{S}_f^j(\tau) = e^{\tau\widehat{H}} S_f^j e^{-\tau\widehat{H}}$, where $\widehat{H}$ is the s–d(f) exchange Hamiltonian (1), and τ the imaginary time varying within interval $(0, 1/T)$ (T is the temperature). The imaginary time ordering operator T_τ arranges all operators on the right side of it in the descending order of the imaginary time τ from left to right. Angle brackets in (3) denote a thermodynamic average over the grand canonical ensemble described by the Hamiltonian $\widehat{H}$.

As is known [7], in the interaction representation: $S_f^j(\tau) = e^{\tau\widehat{H}_0} S_f^j e^{-\tau\widehat{H}_0}$, the expression (3) transforms into:

$$-\langle T_\tau S_f^j(\tau) S_{f'}^{j'}(\tau')\mathfrak{S}(\beta)\rangle_0. \tag{4}$$

Here the scattering matrix $\mathfrak{S}(\beta)$ is defined as:

$$\mathfrak{S}(\beta) = T_\tau \exp\left\{-\int_0^\beta d\tau \widehat{H}_{int}(\tau)\right\}, \tag{5}$$

where in the exponent under the integral the interaction operator (2) is written in the interaction representation. Lower index "0", on the right of the angle brackets in (4) indicates that the thermodynamic averaging is over the ensemble of non-interacting spin and fermion systems. Besides, when expanding the thermodynamic average in (4) using Wick's theorem only connected diagrams should be considered.

The calculation of a T_τ-ordered average of a product of spin S- and fermion c-operators can be divided into two stages: first, only c-operators are coupled, and then the Wick's theorem is applied to the remaining spin operators. Formally this can be written down as follows:

$$\langle T_\tau S_1 \ldots S_l c_1 \ldots c_m^+\rangle_0 = \langle T_\tau S_1 \ldots S_l \langle T_\tau c_1 \ldots c_m^+\rangle_{c0}\rangle_{S0}. \tag{6}$$

Internal thermodynamic average on the right side of Eq. (6) with index "$c0$" denotes averaging only over an ensemble of non-interacting fermions. External T_τ-ordered averaging, indicated by the index "$S0$", should be done using the ensemble of non-interacting spin subsystems. Applying Eq. (6) to the definition of Green's function (4) we can write:

$$-\langle T_\tau S_f^j(\tau) S_{f'}^{j'}(\tau')\mathfrak{S}_S(\beta)\rangle_{S0}, \tag{7}$$

where the effective scattering matrix $\mathfrak{S}_S(\beta)$ is defined by the expression:

$$\mathfrak{S}_S(\beta) = \langle \mathfrak{S}(\beta)\rangle_{c0}. \tag{8}$$

The transformation to the purely spin model is obtained by coupling of all c-operators according to Wick's theorem in each order of the $\mathfrak{S}$-matrix expansion in powers of the coupling constants J. After some, omitted here, diagrammatic and combinatorial calculations it turns out that the result can be presented as a T_τ-ordered exponent:

$$\mathfrak{S}_S(\beta) = T_\tau \exp\{-\Xi\}, \tag{9}$$

where

$$\Xi = \sum_{n=1}^{\infty} \Xi_n,\ \Xi_n = \frac{1}{n}\left(\frac{J}{2}\right)^n \int dx_1 \ldots dx_n G^{(0)}(x_1 - x_2) \times \cdots \times G^{(0)}(x_n - x_1)\mathrm{Sp}\{\widetilde{S}(x_1)\ldots\widetilde{S}(x_n)\}. \tag{10}$$

The functions $G^{(0)}$ in (10) are fermion propagators arising after coupling the c-operators due to Wick's theorem, and the integral over dx_j denotes the operation: $\int_0^\beta d\tau_j \sum_{f_j}$ with $x_j = (\vec{R}_{f_j}, \tau_j)$.

The effective action Ξ describes all possible multi-site spin–spin interactions in the localized spin subsystem in the arbitrary order of the coupling constant J. The partial action Ξ_n determines the n-th order interactions in J and diagrammatically can be represented as a loop with n lines, corresponding to propagators $G^{(0)}$, and n vertices related to spin operators $\widetilde{S}$ (see Fig. 1). It can be seen that all effective interactions in Ξ take into account retardation effects.

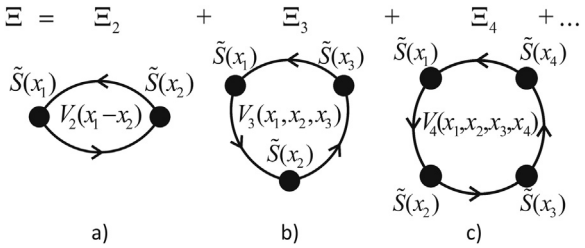

Fig. 1. The effective action Ξ can be expressed as an infinite series of terms Ξ_n. Each term Ξ_n in the diagrammatic representation corresponds to a single loop of n-th order in the exchange coupling constant J and describes the effective n-site spin–spin interaction. The lines with arrows represent bare fermion Green's functions and each vertex, shown with a bold circle, corresponds to a spin operator $\widetilde{S}$.

Note that applied here scheme of integrating over the charge degrees of freedom in the s–d(f) model in some sense is similar to the proof of equivalence between diagrammatic expansion for Green's function of localized f-electrons in the periodic Anderson model and diagrammatic expansion of the fermion Green's function in the Hubbard model [8,9].

4. Effective interactions of the 2nd, 3rd and 4th order in J

Let us consider the first s everal terms of the series for Ξ. The first term with n=1 is zero, because $\mathrm{Sp}\{\widetilde{S}(x_1)\} = \sum_j S^j(x_1)\mathrm{Sp}\{\sigma^j\}$, and $\mathrm{Sp}\{\sigma^j\} = 0$ at any $j = x, y, z$.

To calculate the operator Ξ_2 one should derive the trace $\mathrm{Sp}\{\widetilde{S}(x_1)\widetilde{S}(x_2)\}$. Using the identity: $\sigma^i\sigma^j = \delta_{ij} + i\varepsilon_{ijl}\sigma^l$, where ε_{ijl} is the Levi–Civita antisymmetric tensor we find:

$$\mathrm{Sp}\{\widetilde{S}(x_1)\widetilde{S}(x_2)\} = 2(\vec{S}(x_1)\vec{S}(x_2)). \tag{11}$$

Then the operator Ξ_2 takes the form:

$$\Xi_2 = \int dx_1 dx_2 V_2(x_1 - x_2)\vec{S}(x_1)\vec{S}(x_2), \tag{12}$$

where the effective interaction between spins is defined via a polarization loop (see Fig. 1a):

$$V_2(x_1 - x_2) = \left(\frac{J}{2}\right)^2 G^{(0)}(x_1 - x_2)G^{(0)}(x_2 - x_1). \tag{13}$$

From Eq. (12) it follows that at $f_1 \neq f_2$ the second order effective action Ξ_2 describes indirect exchange interaction of two localized spins through the subsystem of itinerant electrons. However, in contrast to the usual RKKY interaction here the retardation effects, caused by τ-dependence of V_2, are taken into account. Note also that in the Ξ_2 there is a term with $f_1 = f_2$. The Fourier transform of the indirect exchange interaction (13) has the form:

$$V_2(k, i\omega_m) = \left(\frac{J}{2}\right)^2 \chi_0(k, i\omega_m), \tag{14}$$

where

$$\chi_0(k, i\omega_m) = \frac{1}{N}\sum_q \frac{f_q - f_{q+k}}{i\omega_m + \varepsilon_q - \varepsilon_{q+k}} \tag{15}$$

is the Lindhard susceptibility in the Matsubara representation, $\omega_m = 2m\pi T$ with $m \in \mathbb{Z}$, and $f_q = (\exp\{(\varepsilon_q - \mu)/T\} + 1)^{-1}$ is the Fermi–Dirac distribution function. The intensity of the exchange interaction is largely determined by the properties of the itinerant subsystem. The well known RKKY-interaction follows from (15) at $\omega_m \equiv 0$.

Calculating the 3rd order effective action Ξ_3 we obtain (see also Fig. 1b):

$$\Xi_3 = \int dx_1 dx_2 dx_3 V_3(x_1, x_2, x_3) \times \vec{S}(x_1) \cdot (\vec{S}(x_2) \times \vec{S}(x_3)), \quad (16)$$

where

$$V_3(x_1, x_2, x_3) = i\frac{2}{3}\left(\frac{J}{2}\right)^3 G^{(0)}(x_1 - x_2) \times G^{(0)}(x_2 - x_3) G^{(0)}(x_3 - x_1). \quad (17)$$

The formula (16) describes the three-spin interactions in the form of a mixed product of three spin operators. This type of interaction was first considered in [10] but without taking into account the retardation effects.

It is evident that the interaction (16) favors the chiral order in the magnetic subsystem. In this regard we note that in the paper [11] the third order corrections to the Hall conductivity due to s–d(f) exchange interaction were shown to give rise the anomalous Hall effect provided that non-trivial spin configuration (chirality) is formed in the spin subsystem. Interestingly the structure of the expression for the Hall conductivity obtained in [11] is similar to that of (16).

The operator Ξ_4, which determines the effective spin–spin interactions in the fourth order in the coupling constant J, after calculating the trace $\mathrm{Sp}\{\widetilde{S}(x_1)\widetilde{S}(x_2)\widetilde{S}(x_3)\widetilde{S}(x_4)\}$ takes the form (see also Fig. 1c):

$$\Xi_4 = \int dx_1 dx_2 dx_3 dx_4 V_4(x_1, x_2, x_3, x_4) \times (\vec{S}(x_1)\vec{S}(x_2)) \cdot (\vec{S}(x_3)\vec{S}(x_4)), \quad (18)$$

where

$$\begin{aligned} V_4(x_1, x_2, x_3, x_4) = \frac{1}{2}\left(\frac{J}{2}\right)^4 [&G^{(0)}(x_1 - x_2) \times G^{(0)}(x_2 - x_3) G^{(0)}(x_3 - x_4) \\ &\times G^{(0)}(x_4 - x_1) - G^{(0)}(x_1 - x_3) G^{(0)}(x_3 - x_2) G^{(0)}(x_2 - x_4) \\ &\times G^{(0)}(x_4 - x_1) + G^{(0)}(x_1 - x_4) \\ &\times G^{(0)}(x_4 - x_3) G^{(0)}(x_3 - x_2) G^{(0)}(x_2 - x_1)]. \end{aligned} \quad (19)$$

The terms of the expression (18) with unequal indices of sites f_j ($j = 1, \ldots, 4$) correspond to the four-spin exchange interactions. Among them there are, in particular, interactions describing ring exchange of four spins located, for example, at the square plaquette vertices. For the first time the ring exchange (without retardation effects) was obtained from the Hubbard model at half filling in the fourth order of the perturbation theory in the parameter t/U, where t is the tunneling integral, and U is the Coulomb repulsion energy of two electrons at the same site [12]. The four-spin ring exchange interaction was involved to explain the magnetic ordering features in the quantum crystal ^{3}He [13]. In the paper [14] it was argued that ring exchange is important to describe magnetic properties of cuprate high-temperature superconductors. Effect of ring exchange interaction on the superconductivity in cuprates was investigated in [15].

At pairwise coincident site indices: $f_3 = f_1$ and $f_4 = f_2$, in the sum (18) there are terms that are responsible for biquadratic exchange interaction. These interactions were first used in [16] for explaining the paramagnetic resonance on Mn ions in the compound MnO. Besides, the biquadratic exchange interaction is essential in multilayer magnetic systems [17].

5. Conclusion

The paper presents a method of deriving all possible kinds of effective indirect interactions between the localized spins due to s–d(f) exchange coupling of these spins with the subsystem of itinerant electrons. After integrating over the charge degrees of freedom in the s–d(f) exchange model an exact representation for an action of a purely spin model is obtained. Using this action allows to study the spin subsystem in the s–d(f) model in the framework of effective purely spin model. The important point of this model is that all effective interactions take into account retardation effects. Although explicit expressions are written only for two-, three- and four-spin interactions, the formula (10) allows to generate multi-site spin–spin interactions in the arbitrary order in the s–d(f) exchange coupling constant J.

The validity of the suggested theory is, obviously, restricted by the smallness of the s–d(f) exchange interaction as compared to the conduction bandwidth. Otherwise, we are not allowed to be confined by the study only the lowest orders (in J) of effective interactions but the entire series (10) should be considered. The need to sum up the entire series makes the advantages of the proposed approach not so obvious. Besides, we should keep in mind that in real materials the wave functions of itinerant and localized electrons are not orthogonal. Mathematically this is reflected in noncommutativity of the Fermi and quasi-spin operators, which significantly complicates the application of the diagram technique [18,19]. As a result, the shown in the article formulas for the effective action cease to be valid. The last remark, however, concerns rather model used in the work then the suggested method.

Within the s–d(f) model, involving orthogonality of the s- and d(f)-states, in the regime where J is not greater than the conduction bandwidth, the proposed approach opens up new opportunities for the study of various magnetic phases in the systems with itinerant electrons. As was already noted the third order interactions (16) may lead to the helical magnetic structures and the fourth order interactions (18) explain particularly the occurrence of ring exchange and biquadratic exchange interactions. Also our theory suggests a relatively simple way to investigate the influence of retardation effects in the indirect exchange interactions on the phase diagram of the systems with itinerant electrons.

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