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Renormalization Group Approach for the Double Exchange Ferromagnets

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The discovery of the colossal magnetoresistance (CMR) in the manganese oxides with perovskite structures $T_{1-x}DMnO_3$ ($T = La, Pr, Nd$; $D = Sr, Ca, Ba, Pb$) and its potential technological application motivated theoretical and experimental researchers to study the itinerant ferromagnetism. A first theoretical description of this phenomenon in terms of the double-exchange mechanism was given a long time ago by Zener. In this model, the spin orientation of adjacent Mn-moments is associated with kinetic exchange of conduction e_g electrons. Consequently, alignment of the core Mn-spins by an external magnetic field causes higher conductivity. The Mn ions are considered as localized forming a spin of $S = \frac{3}{2}$ and they are coupled to the itinerant electrons by a strong ferromagnetic Hund coupling, $J_H > 0$. We apply the flow equation technique (nonperturbative method, based on continuous canonical transformation) to the double-exchange model for ferromagnetism described by the Kondo type Hamiltonian. We want to eliminate the interaction term responsible for non-conservation of magnon number and to take into account fermion and magnon degrees of freedom. We express the spin operators of Mn ions via the magnon operators (the Holstein-Primakoff transformation) and investigate the magnon excitation spectrum determined by Green's function.

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1. Introduction

Due to discovery of the colossal magnetoresistance and its potential application in information technology or spintronic the understanding of itinerant ferromagnetism [1, 2] of manganese oxides is a challenge for scientists. So far, some magnetic properties has been studied by investigating the magnon spectrum at non-Ruderman-Kittel-Kasuya-Yosida (non-RKKY) indirect exchange in conducting ferromagnets [3], in spin wave theory of double exchange ferromagnets [4], by application of continuous canonical transformation [5] and slave fermion approach to the quantum double-exchange (DEX) model [6], by analysis of on-site Hubbard repulsion effects [7] and interacting spin waves in the ferromagnetic Kondo lattice model [8], etc. Also Monte Carlo scheme of enhanced ferromagnetism from electron-electron interactions in double exchange models [9] has been considered.

In this paper we want to study physics of the DEX ferromagnets applying continuous unitary transformation. So-called flow equation approach introduced in 1994 by Wegner [10] in the context of condensed matter theory and independently by Wilson with Głazek [11] in the high energy physics proved to be very useful nonperturbative approach for studying a number of problems in the condensed matter physics [12]. This method originates from the renormalization group technique. The flow equation scheme involves unconventional scaling and retains the full Hilbert space, so we keep information on all energy scales of our systems. Such process is based on a continuous diagonalization of the relevant Hamiltonian which is ultimately reduced to a diagonal (or block-diagonal) structure via the set of infinite transformation. The uni-

tary flow of the Hamiltonian is generated by the anti-Hermitian operator. Particular choice of this canonical generator depends on the subtleties of the considered problem [12]. We have applied such unitary transformations for BCS superconductors [13] and for the systems of coherent and incoherent preformed pairs [14]. Now, we shall try to extend such algorithm for the strong ferromagnetic coupling limit which is relevant to the manganites.

2. The double exchange model

The DEX model for ferromagnetism is described by the Kondo type Hamiltonian [15]:

$$\hat{H} = \sum_{\mathbf{k}, \sigma} (\varepsilon_{\mathbf{k}} - \mu) \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} - J_H \sum_{i, \sigma, \sigma'} (\hat{S}_i \hat{s}_i)^{\sigma\sigma'} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma'}, \quad (1)$$

where $\hat{c}_{\mathbf{k}\sigma}^\dagger$ ($\hat{c}_{\mathbf{k}\sigma}$) is creation (annihilation) operators of the conduction e_g electrons, $\varepsilon_{\mathbf{k}}$ are the energies of e_g , μ is chemical potential, \hat{s}_i — spin operators of e_g , \hat{S}_i — spin operators of Mn ions, $J_H > 0$ is the Hund coupling (for manganites known to be very large) and characterizes local ferromagnetic interaction. Let us represent the spin operators of Mn ions \hat{S}_i via the magnon operators \hat{b}_i^\dagger , \hat{b}_i (the Holstein-Primakoff transformation): $\hat{S}_i^- = \hat{b}_i^\dagger (2S - \hat{b}_i^\dagger \hat{b}_i)^{\frac{1}{2}}$, $\hat{S}_i^+ = (\hat{S}_i^-)^\dagger$, $\hat{S}_i^z = S - \hat{b}_i^\dagger \hat{b}_i$, where $S = \frac{3}{2}$. Magnon operators \hat{b}_i^\dagger , \hat{b}_i obey the boson commutation relations. By simplifying spin operators: $\hat{S}_i^- = \hat{b}_i^\dagger \sqrt{2S}$, $\hat{S}_i^+ = \hat{b}_i \sqrt{2S}$ (it is true at low temperatures) and using the Pauli operators for e_g electron spins we can rewrite the model Hamiltonian as

$$\begin{aligned} \hat{H} &= \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}^{\sigma} \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \hat{b}_{\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{q}} \\ &+ \frac{J_{\text{H}}}{2N} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} \hat{b}_{\mathbf{p}+\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{p}} (\hat{c}_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} \hat{c}_{\mathbf{k}\uparrow} - \hat{c}_{\mathbf{k}-\mathbf{q}\downarrow}^{\dagger} \hat{c}_{\mathbf{k}\downarrow}) \\ &- J_{\text{H}} \sqrt{\frac{S}{2N}} \sum_{\mathbf{k},\mathbf{q}} (\hat{b}_{\mathbf{q}}^{\dagger} \hat{c}_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} \hat{c}_{\mathbf{k}\downarrow} + \text{H.c.}), \end{aligned} \quad (2)$$

where $\xi_{\mathbf{k}}^{\sigma} = \varepsilon_{\mathbf{k}} - \mu^{\sigma}$, $\mu^{\uparrow} = \mu + \frac{1}{2}SJ_{\text{H}}$, $\mu^{\downarrow} = \mu - \frac{1}{2}SJ_{\text{H}}$ and the last term in (2) describes the double exchange interaction.

3. Formulation of the flow equations

3.1. Diagonalization of the Hamiltonian

The model Hamiltonian can be split up in a diagonal and interaction part

$$\hat{H}(l) = \hat{H}_0(l) + \hat{H}_{\text{int}}(l), \quad (3)$$

where [5]

$$\hat{H}_{\text{int}}(l) = -\frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} (I_{\mathbf{k},\mathbf{q}}(l) \hat{b}_{\mathbf{q}}^{\dagger} \hat{c}_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} \hat{c}_{\mathbf{k}\downarrow} + \text{H.c.}) \quad (4)$$

and

$$\begin{aligned} \hat{H}_0(l) &= \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}^{\sigma} \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \hat{b}_{\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{q}} \\ &+ \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'} \delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}'} \left[U_{\mathbf{k},\mathbf{q},\mathbf{q}',\mathbf{k}'} \hat{c}_{\mathbf{k}\downarrow}^{\dagger} \hat{c}_{\mathbf{q}\uparrow}^{\dagger} \hat{c}_{\mathbf{q}'\uparrow} \hat{c}_{\mathbf{k}'\downarrow} \right. \\ &+ \hat{b}_{\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{q}'} \left(M_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'}^{\uparrow}(l) \hat{c}_{\mathbf{k}\uparrow}^{\dagger} \hat{c}_{\mathbf{k}'\uparrow} \right. \\ &\left. \left. - M_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'}^{\downarrow}(l) \hat{c}_{\mathbf{k}\downarrow}^{\dagger} \hat{c}_{\mathbf{k}'\downarrow} \right) \right] + \delta H_0(l). \end{aligned} \quad (5)$$

Initial conditions ($l = 0$) for the model parameters: $\xi_{\mathbf{k}}^{\sigma}(0) = \varepsilon_{\mathbf{k}} - \mu^{\sigma}$, $I_{\mathbf{k},\mathbf{q}}(0) = J_{\text{H}} \sqrt{\frac{S}{2}}$, $M_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'}^{\sigma}(0) = \frac{J_{\text{H}}}{2}$, $U_{\mathbf{k},\mathbf{q},\mathbf{q}',\mathbf{k}'}(0) = 0$. We choose the canonical operator $\eta(l) = [\hat{H}_0(l), \hat{H}_{\text{int}}(l)]$ [10] which is given by

$$\hat{\eta}(l) = -\frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} \alpha_{\mathbf{k},\mathbf{q}}(l) (I_{\mathbf{k},\mathbf{q}}(l) \hat{b}_{\mathbf{q}}^{\dagger} \hat{c}_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} \hat{c}_{\mathbf{k}\downarrow} - \text{H.c.}), \quad (6)$$

where $\alpha_{\mathbf{k},\mathbf{q}}(l) = \xi_{\mathbf{k}-\mathbf{q}}^{\uparrow}(l) - \xi_{\mathbf{k}}^{\downarrow}(l)$. Transformation of the Hamiltonian $\hat{H}(l)$ proceeds as long as $\eta(l)$ is finite, which occurs until $I_{\mathbf{k},\mathbf{q}}(l) \rightarrow 0$. This is achieved in the asymptotic limit $l \rightarrow \infty$.

The set of flow equations for parameters of the DEX model Hamiltonian is given by [5]:

$$\frac{dI_{\mathbf{k},\mathbf{q}}(l)}{dl} = -\alpha_{\mathbf{k},\mathbf{q}}^2(l) I_{\mathbf{k},\mathbf{q}}(l), \quad (7)$$

$$\frac{d\xi_{\mathbf{k}}^{\downarrow}(l)}{dl} = -\frac{2}{N} \sum_{\mathbf{q}} \alpha_{\mathbf{k},\mathbf{q}}(l) |I_{\mathbf{k},\mathbf{q}}(l)|^2 \quad (8)$$

and additional for $U(l)$ and $M(l)$. In the lowest order estimation

$$\begin{aligned} I_{\mathbf{k},\mathbf{q}}(l) &= I_{\mathbf{k},\mathbf{q}}(0) e^{-\alpha_{\mathbf{k},\mathbf{q}}^2 l} \\ &= J_{\text{H}} \sqrt{\frac{S}{2}} e^{-(\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow})^2 l}, \end{aligned} \quad (9)$$

$$\xi_{\mathbf{k}}^{\downarrow}(\infty) = \xi_{\mathbf{k}}^{\downarrow} - \frac{J_{\text{H}}^2 S}{2} \sum_{\mathbf{q}} \frac{1}{\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow}}. \quad (10)$$

For more details see [5].

3.2. Magnon energy spectrum

From the initial derivative in ($l = 0$) we find that

$$\left(\frac{d\hat{b}_{\mathbf{q}}^{\dagger}(l)}{dl} \right)_{l=0} = [\hat{\eta}(l), \hat{b}_{\mathbf{q}}^{\dagger}(l)]_{l=0}, \quad (11)$$

where $\hat{b}_{\mathbf{q}}^{\dagger}(0) = \hat{b}_{\mathbf{q}}^{\dagger}$ and $\hat{b}_{\mathbf{q}}(0) = \hat{b}_{\mathbf{q}}$. Using the generating operator (6) we calculate the flow of magnon operator

$$\begin{aligned} \left(\frac{d\hat{b}_{\mathbf{q}}^{\dagger}(l)}{dl} \right)_{l=0} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \alpha_{\mathbf{k},\mathbf{q}}(0) I_{\mathbf{k},\mathbf{q}}(0) \hat{c}_{\mathbf{k}\downarrow}^{\dagger} \hat{c}_{\mathbf{k}-\mathbf{q}\uparrow}, \\ \left(\frac{d\hat{b}_{\mathbf{q}}(l)}{dl} \right)_{l=0} &= \left(\frac{d\hat{b}_{\mathbf{q}}^{\dagger}(l)}{dl} \right)_{l=0}^{\dagger}. \end{aligned} \quad (12)$$

From Eq. (12) we conclude the following l -dependent parameterization of the magnon operators

$$\begin{aligned} \hat{b}_{\mathbf{q}}^{\dagger}(l) &= A_{\mathbf{q}}(l) \hat{b}_{\mathbf{q}}^{\dagger} + \sum_{\mathbf{k}} B_{\mathbf{k},\mathbf{q}}(l) \hat{c}_{\mathbf{k}\downarrow}^{\dagger} \hat{c}_{\mathbf{k}-\mathbf{q}\uparrow}, \\ \hat{b}_{\mathbf{q}}(l) &= (\hat{b}_{\mathbf{q}}^{\dagger}(l))^{\dagger}, \end{aligned} \quad (13)$$

with the initial boundary conditions $A_{\mathbf{q}}(0) = 1$ and $B_{\mathbf{k},\mathbf{q}}(0) = 0$. We next use the ansatz (13) in the flow equation for the magnon operator $\frac{d\hat{b}_{\mathbf{q}}^{\dagger}(l)}{dl} = [\hat{\eta}(l), \hat{b}_{\mathbf{q}}^{\dagger}(l)]$. On this basis we obtain the following set of flow equations for l -dependent coefficients

$$\frac{dA_{\mathbf{q}}(l)}{dl} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \alpha_{\mathbf{k},\mathbf{q}}(l) I_{\mathbf{k},\mathbf{q}}(l) [n_{\mathbf{k}}^{\downarrow} - n_{\mathbf{k}-\mathbf{q}}^{\uparrow}] B_{\mathbf{k},\mathbf{q}}(l), \quad (14)$$

$$\frac{dB_{\mathbf{k},\mathbf{q}}(l)}{dl} = \frac{1}{\sqrt{N}} \alpha_{\mathbf{k},\mathbf{q}}(l) I_{\mathbf{k},\mathbf{q}}(l) A_{\mathbf{q}}(l), \quad (15)$$

where $n_{\mathbf{k}}^{\sigma} = [\exp(\xi_{\mathbf{k}}^{\sigma}/k_{\text{B}}T) + 1]^{-1}$ is the Fermi–Dirac distribution function. By investigating (14) and (15) in the lowest order solution we find that

$$\begin{aligned} A_{\mathbf{q}}(l) &= \frac{J_{\text{H}}^2 S}{4N} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}}^{\downarrow} - n_{\mathbf{k}-\mathbf{q}}^{\uparrow}}{(\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow})^2} \\ &\times \left(\exp(-2(\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow})^2 l) \right. \\ &\left. - 2 \exp(-(\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow})^2 l) + 1 \right), \end{aligned} \quad (16)$$

$$B_{\mathbf{k},\mathbf{q}}(l) = -\frac{1}{\sqrt{N}} \frac{I_{\mathbf{k},\mathbf{q}}(l) - I_{\mathbf{k},\mathbf{q}}(0)}{\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow}}. \quad (17)$$

Their asymptotic values ($l \rightarrow \infty$) have the following structure:

$$\tilde{A}_{\mathbf{q}} = 1 - \frac{J_{\text{H}}^2 S}{4N} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}-\mathbf{q}}^{\uparrow} - n_{\mathbf{k}}^{\downarrow}}{(\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow})^2}, \quad (18)$$

$$\tilde{B}_{\mathbf{k},\mathbf{q}} = J_{\text{H}} \sqrt{\frac{S}{2N}} \frac{1}{\xi_{\mathbf{k}-\mathbf{q}}^{\uparrow} - \xi_{\mathbf{k}}^{\downarrow}}. \quad (19)$$

The excitation spectrum can be determined from the magnon Green function $\langle\langle \hat{b}_{\mathbf{q}}; \hat{b}_{\mathbf{q}}^{\dagger} \rangle\rangle_{\hat{H}}$. Taking into account the statistical averages of the observables and the invariance of trace on the unitary transformation we can write

$\langle\langle \hat{b}_q; \hat{b}_q^\dagger \rangle\rangle_{\hat{H}} = \langle\langle \hat{b}_q(l); \hat{b}_q^\dagger(l) \rangle\rangle_{\hat{H}(l)} = \langle\langle \hat{b}_q(\infty); \hat{b}_q^\dagger(\infty) \rangle\rangle_{\hat{H}(\infty)}$
 which is explicitly given by

$$\begin{aligned} & \langle\langle \hat{b}_q(\infty); \hat{b}_q^\dagger(\infty) \rangle\rangle_{\hat{H}(\infty)} \\ &= \left\langle\left\langle \tilde{A}_q^* \hat{b}_q + \sum_{\mathbf{k}} \tilde{B}_{\mathbf{k},q}^* \hat{c}_{\mathbf{k}-q\uparrow}^\dagger \hat{c}_{\mathbf{k}\downarrow}; \tilde{A}_q \hat{b}_q^\dagger \right.\right. \\ &+ \left.\left. \sum_{\mathbf{k}'} \tilde{B}_{\mathbf{k}',q} \hat{c}_{\mathbf{k}'\downarrow}^\dagger \hat{c}_{\mathbf{k}'-q\uparrow} \right\rangle\right\rangle \\ &= |\tilde{A}_q|^2 \langle\langle \hat{b}_q; \hat{b}_q^\dagger \rangle\rangle \\ &+ \sum_{\mathbf{k}, \mathbf{k}'} \tilde{B}_{\mathbf{k},q}^* \tilde{B}_{\mathbf{k}',q} \langle\langle \hat{c}_{\mathbf{k}-q\uparrow}^\dagger \hat{c}_{\mathbf{k}\downarrow}; \hat{c}_{\mathbf{k}'\downarrow}^\dagger \hat{c}_{\mathbf{k}'-q\uparrow} \rangle\rangle \\ &= |\tilde{A}_q|^2 \frac{1}{\omega - \tilde{\omega}_q} + \sum_{\mathbf{k}} |\tilde{B}_{\mathbf{k},q}|^2 \frac{n_{\mathbf{k}-q}^\uparrow - n_{\mathbf{k}}^\downarrow}{\omega + \tilde{\xi}_{\mathbf{k}-q}^\uparrow - \tilde{\xi}_{\mathbf{k}}^\downarrow}. \quad (20) \end{aligned}$$

Magnon spectral function is determined by the imaginary part of the Green function $\rho(q, \omega) = -\frac{1}{\pi} \Im \langle\langle \hat{b}_q; \hat{b}_q^\dagger \rangle\rangle_{\omega+i0^+}$.

4. Summary

In this paper we construct the continuous unitary transformation for the DEX model. We present how the flow equation method works and how the energy spectrum appears in this regime. As one can see in Fig. 1, magnon spectrum consists of the coherent (long-lived) and incoherent (damped) part. These branches are separated by a fairly large energy. Contribution of the coherent part is about 60–70 percent (see Fig. 2). Due to small occupancy of the incoherent part appearing at high energies its influence on physical properties could be negligible.

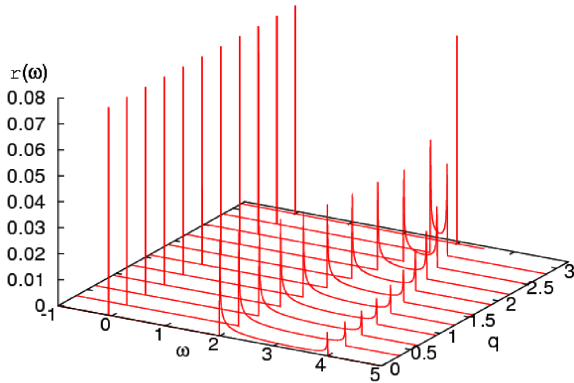


Fig. 1. The effective spectrum of magnons.

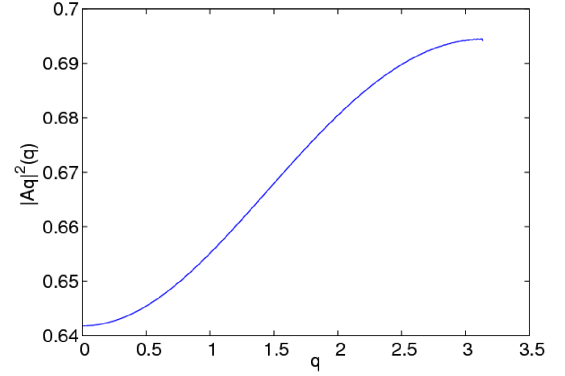


Fig. 2. Contribution of the long-lived magnon excitations.

The next step will contain analytical and numerical development of the project and comparison of our estimation to other theoretical and experimental results.

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