Continuous canonical transformation
for the double exchange model

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Abstract

The method of continuous canonical transformation is applied to the double exchange model with a purpose to eliminate the interaction term responsible for non conservation of magnon number. Set of differential equations for the effective Hamiltonian parameters is derived. Within the lowest order (approximate) solution we reproduce results of the standard (single step) canonical transformation. Results of the selfconsistent numerical treatment are compared with the other known studies for this model.

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I. INTRODUCTION

The discovery of colossal magnetoresistance in the doped manganites attracted new interests in studying itinerant ferromagnetism phenomena. The double exchange model (DEX), introduced a long time ago [1,2], seems to be a good starting point to explain the paramagnetic - ferromagnetic transition. Conduction \( eg \) electrons interact via the strong Hund’s coupling with the localized Mn ions (their spin being \( S = 3/2 \)). This interaction drives the core Mn spins to ferromagnetic alignment, owing to the kinetic processes of itinerant electrons. Whether the DEX scenario itself is enough for an explanation of magnetoresistance in manganites, or should be supplemented by other realistic effects like e.g. lattice Jahn-Teller distortions [3], competition with the superexchange [4,5] and strong Coulomb interactions between electrons [6], is an open question under discussion.

In this paper we want to reexamine physics of the DEX model using the renormalization group approach in a version proposed recently by Wegner [7] and independently by Glazek and Wilson [8]. This procedure known as the flow equation method has proved to be a powerful tool, especially for analysis of models composed of several coupled subsystems. So far, it has been successfully applied to the problem of electron - phonon interaction [9] (where the Fröhlich transformation has been revised), the single impurity Anderson model [10], the spin - boson model for dissipative systems [11], the spin - polaron coupling for \( t-J \) model [12], DEX model in the RKKY (small coupling) limit [13], and the charge exchange interaction for the boson - fermion model [14]. The same method has also been used for studying effects of correlations, e.g. in the Hubbard model [15] (\( t/U \) expansion), the large spin Heisenberg Hamiltonian [16] (1/\( S \) expansion), etc. Recently there has been proposed a highly sophisticated computer aided perturbation method based on the flow equation technique to study the dimerized spin models [17]. It is our belief, that the flow equation technique can be a reliable source of information also for the DEX model. In particular we would like to consider the strong (ferromagnetic) coupling limit (relevant for manganites) and compare our results to other studies of this model.
The DEX model for ferromagnetism is described by the Kondo type Hamiltonian

\[ H = \sum_{k,\sigma} \left( \varepsilon_k - \mu \right) c_{k\sigma}^{\dagger} c_{k\sigma} - J_H \sum_{i,\sigma,\sigma'} (S_i^s S_i^{s'}) c_{i\sigma}^{\dagger} c_{i\sigma'} \]  

(1)

where \( c_{k\sigma}^{\dagger} \) correspond to annihilation (creation) operators of the conduction \( e_g \) electrons, \( s_i \) denotes their spin operators and \( S_i \) stands for the spin operator of Mn ions. Local ferromagnetic interaction is characterized by the Hund’s coupling \( J_H > 0 \), for manganites known to be very large. With a help of the Holstein-Primakoff transformation we can represent the spin operators \( S_i \) via the magnon operators \( a_i^{\dagger}, a_i \) such that

\[ S_i^- = a_i^{\dagger} (2S - a_i^{\dagger} a_i)^{1/2}, \quad S_i^+ = (S_i^-)^{\dagger}, \quad S_i^z = S - a_i^{\dagger} a_i. \]

Magnon operators \( a_i^{\dagger}, a_i \) obey the boson (commutation) relations.

At sufficiently low temperatures the system is close to ferromagnetic (ground state) ordering, so we can simplify spin operators to

\[ S_i^z \approx a_i^{\dagger} \sqrt{2S}, \quad S_i^+ \approx a_i \sqrt{2S}. \]

Using the Pauli operators for \( e_g \) electron spins one gets the model Hamiltonian in a following form

\[ H = \sum_{k,\sigma} \xi_k^{\sigma} c_{k\sigma}^{\dagger} c_{k\sigma} + \frac{J_H}{2N} \sum_{q,p,k} a_{p+q}^{\dagger} a_p \left( c_{k-q}^{\dagger} c_{k}^{\dagger} - c_{k-q}^{\dagger} c_{k}^{\dagger} \right) \]

\[ - J_H \sqrt{\frac{S}{2N}} \sum_{q,k} \left( a_{q}^{\dagger} c_{k-q}^{\dagger} c_{k}^{\dagger} + \text{h.c.} \right), \]

(2)

with \( \xi_k^{\sigma} = \varepsilon_k - \mu^{\sigma} \) and \( \mu^\uparrow = \mu + \frac{1}{2} SJ_H, \mu^\downarrow = \mu - \frac{1}{2} SJ_H \). If temperature is comparable with \( J_H/k_B \) then one should include the higher order terms in the square root expansion \( \sqrt{1 - (a_i^{\dagger} a_i/2S)} \) for magnon operators.

In what follows, we design the unitary transformation to eliminate last part of the Hamiltonian (2) linear in \( a_q^{(1)} \) operators, which is responsible for a violation of the magnon number \( \sum_i < a_i^{\dagger} a_i > \). To the leading order of \( 1/S \) one can eliminate this exchange interaction using a single step canonical transformation \( e^A H e^{-A} \) with the generating operator \( A \) given by

\[ A = J_H \sqrt{\frac{S}{2N}} \sum_{k,q} \left( a_{q}^{\dagger} c_{k-q}^{\dagger} c_{k}^{\dagger} - \xi_k^{\dagger} - \xi_k - \text{h.c.} \right). \]

(3)

However, this transformation generates a whole lot of higher order interactions, their amplitudes being eventually not negligible. Recently it has been shown by means of the standard
perturbation treatment [20] that these interactions give rise to quantum corrections for spin wave spectrum (both for dispersion and the life time effects). That such corrections are in fact important it is known independently from the direct numerical studies of finite chains [21] and from analysis based on the variational wave functions [22].

Instead of the single step transformation (3) we propose in this paper a different method using an infinite sequence of the infinitesimal transformations what gives us more control for a derivation of the required effective Hamiltonian. In particular, we want the higher order many-body interactions to be as small as possible, thus being more tractable via the standard perturbation study.

In the following section we give a brief introduction to the method of continuous transformation and derive the corresponding flow equations for parameters of the DEX model. Next, we discuss an analytical approximate solution of these equations and compare it with results of the standard single step transformation. In the last part we present the selfconsistent numerical solution for the model parameters along with some rough estimation of the spin stiffness coefficient.

II. FORMULATION OF FLOW EQUATIONS

A main idea of the method is to transform the initial Hamiltonian $H$ through the series of unitary transformations $H(l) = U(l)HU^\dagger(l)$, labeled with some continuous flow parameter $l$. In a course of transformation the Hamiltonian evolves according to the following flow equation

$$\frac{dH(l)}{dl} = [\eta(l), H(l)], \quad (4)$$

where the generator $\eta(l)$ is related to $U(l)$ via $\eta(l) = (dU(l)/dl)U^\dagger(l)$. This operator has to be chosen depending on a purpose of the transformations. Wegner has shown [4] that with $\eta(l) = [H(l) - H_{\text{int}}(l), H(l)]$ one can eventually eliminate the (perturbation) part of the Hamiltonian $H_{\text{int}}(l \to \infty) = 0$, provided that no degenerate states are encountered.
Alternative choice for \( \eta \), efficient even in a presence of degeneracies, has been proposed recently by Mielke [23]. In this work we use the slightly modified Wegner’s proposal for \( \eta(l) \).

To be specific, we define the interaction part as

\[
H_{\text{int}}(l) = \frac{-1}{\sqrt{N}} \sum_{k,q} \left( I_{k,q}(l) a_{q,k-q}^{\dagger} c_{k} + \text{h.c.} \right).
\]

(5)

The remaining part \( H_0(l) = H(l) - H_{\text{int}}(l) \) may contain not only the other two terms of (2) but additionally also contributions induced by transformation for \( l > 0 \). To take these into account we assume \( H_0(l) \) to have the following structure

\[
H_0(l) = \sum_{k,\sigma} \xi_k^\sigma(l) c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{N} \sum_{k,k',q,q'} \delta_{k+q,k'+q'} \left[ U_{k,q,k',q'}(l) c_{k}^{\dagger} c_{q}^{\dagger} c_{k'} c_{q'} \right]
+ \left( M_{k,k',q,q'}(l) c_{k}^{\dagger} c_{k'} c_{q}^{\dagger} c_{q'} + M_{k,k',q,q'}^{\ast}(l) c_{k}^{\dagger} c_{q}^{\dagger} c_{k'} c_{q'} + \text{h.c.} \right)
\]

(6)

where \( \delta H_0(l) \) contains all types of interactions not shown explicitly in (3). The initial conditions for the model parameters read

\[
\xi_k^\sigma(0) = \varepsilon_k - \mu^\sigma, \quad U_{k,q,k',q'}(0) = 0, \quad I_{k,q}(0) = J_H \sqrt{\frac{S}{2}}, \quad M_{k,k',q,q'}(0) = \frac{J_H}{2}.
\]

(7)

(8)

We choose the generating operator \( \eta(l) = [\sum_{k,\sigma} \xi_k^\sigma(l) c_{k\sigma}^\dagger c_{k\sigma}, H_{\text{int}}(l)] \) which explicitly is given by

\[
\eta(l) = \frac{-1}{\sqrt{N}} \sum_{k,q} \alpha_{k,q}(l) \left( I_{k,q}(l) a_{q,k-q}^{\dagger} c_{k} + \text{h.c.} \right),
\]

(9)

where \( \alpha_{k,q}(l) = \xi_{k-q}^\dagger(l) - \xi_k^\dagger(l) \). Notice, that (9) has similar structure to the generating operator \( A \) of the standard transformation (3).

Using the general flow equation (11) we obtain

\[
\frac{dH(l)}{dl} = \frac{1}{\sqrt{N}} \sum_{k,q} \left( \alpha_{k,q}(l) \right)^2 \left( I_{k,q}(l) a_{q,k-q}^{\dagger} c_{k} + \text{h.c.} \right) - \frac{2}{N} \sum_{k,q} \alpha_{k,q}(l) |I_{k,q}(l)|^2 c_{k}^{\dagger} c_{k} + 
+ \frac{1}{N} \sum_{k,k',q,q'} \left( \alpha_{k,q}(l) + \alpha_{k',q'}(l) \right) I_{k,q}(l) I_{k',q'}^{\ast}(l) \left[ a_{q}^{\dagger} a_{q'} \left( c_{k-q}^{\dagger} c_{k'-q'} + \delta_{k,k'} \right)
- c_{k}^{\dagger} c_{k} \delta_{k-q,k'-q'} \right]
+ \left[ \eta(l), \delta H_0(l) \right] + O(IM) + O(IU).
\]

(10)
Terms of the order $I(l)M(l)$, $I(l)U(l)$ are symbolically denoted as $O(IM)$ and $O(IU)$. If they were included in the diagonal part through $\delta H_0(l)$ they would induce some higher order interactions given by $[\eta(l),\delta H_0(l)]$.

Equation (10) is a differential flow equation for the Hamiltonian which has to be solved. In the next section we solve it approximately neglecting the last three terms on the right hand side.

III. LOWEST ORDER SOLUTION

It is instructive to study first the flow equation (10) with the last three terms on the right hand side omitted. It means that we neglect the interactions expressed by more than four operators, i.e. scattering between more than two particles. On a level of this assumption one may expect that effective Hamiltonian should differ from its initial form by some correction comparable with $H'_2$ of the Ref. [20]. The set of the flow equations for parameters of the DEX model Hamiltonian is simply given by

$$\frac{dI_{k,q}(l)}{dl} = -\alpha_{k,q}(l)I_{k,q}(l),$$

$$\frac{\xi_{k}^\uparrow(l)}{dl} = -\frac{2}{N} \sum_q \alpha_{k,q}(l)|I_{k,q}(l)|^2,$$

$$\frac{dU_{k,p,p',k'}(l)}{dl} = (\alpha_{k',p'\rightarrow p}(l) + \alpha_{k,k\rightarrow p'}(l)) I_{k',p'-p}(l)I_{k,k-p'}^*(l),$$

$$\frac{M_{k,k',q,q'}^{\uparrow}(l)}{dl} = (\alpha_{k+q,q}(l) + \alpha_{k',q'\rightarrow q}(l)) I_{k+q,q}(l)I_{k',q'+q'}^*(l),$$

$$\frac{M_{k,k',q,q'}^{\downarrow}(l)}{dl} = (\alpha_{k',q}(l) + \alpha_{k,q'}(l)) I_{k',q}(l)I_{k,q'}^*(l).$$

There is no renormalization for spin $\sigma = \uparrow$ electrons, so $\xi_{k}^{\uparrow}(l) = \xi_{k}^{\uparrow}$. Still, the set of flow equations (11-15) is impossible to solve by other than numerical way. To get some insight in a process of the continuous transformation for $H(l)$ we assume further that the energy $\xi_{k}^{\downarrow}(l)$ is only weakly affected by renormalization. We verified validity of such assumption by solving selfconsistently the flow equations numerically for one dimensional tight binding electron dispersion (see the next section). We thus can drop $l$ dependence...
of the parameter $\alpha_{k,q}(l)$ on the right hand side of flow equations. One easily obtains an
analytical solution for a flow of the exchange coupling

$$I_{k,q}(l) = I_{k,q}(0)e^{-\alpha_{k,q}^2l} = J_H\sqrt{\frac{S}{2}}e^{-(\xi_{k,q}^\uparrow-\xi_{k,q}^\downarrow)^2l}. \quad (16)$$

In the limit $l \to \infty$ the exchange coupling drops asymptotically to zero and so does the part
(5) of the Hamiltonian, $H_{\text{int}}(l \to \infty) = 0$.

Determination of the other $l$-dependent parameters, such as $\xi_{k,q}^\downarrow(l)$, $U(l)$ and $M^\sigma(l)$ is
straightforward. We summarize our results by showing values of these parameters in the
limit $l \to \infty$

$$\xi_{k,q}^\downarrow(\infty) = \xi_{k,q} - \frac{J_H^2S}{2} \sum_q \frac{1}{\xi_{q}^\downarrow - \xi_{k,q}^\downarrow}, \quad (17)$$

$$U_{k,p,p',k'}(\infty) = \frac{J_H^2S}{2} f_{p,k',p',k} \quad (18)$$

$$M_{k,k',q,q'}^{\uparrow}(\infty) = \frac{J_H^2S}{2} + \frac{J_H^2S}{2} f_{k,k+q,k',k'+q'}, \quad (19)$$

$$M_{k,k',q,q'}^{\downarrow}(\infty) = \frac{J_H^2S}{2} + \frac{J_H^2S}{2} f_{k'-q,k'-k',k'}, \quad (20)$$

where

$$f_{1,2,3,4} = \frac{\xi_{1}^\downarrow - \xi_{2}^\downarrow + \xi_{3}^\downarrow - \xi_{4}^\downarrow}{(\xi_{1}^\downarrow - \xi_{2}^\downarrow)^2 + (\xi_{3}^\downarrow - \xi_{4}^\downarrow)^2}. \quad (21)$$

Using the standard canonical transformation (3) one obtains the same scaling for the pa-
rameters (17-20) but with a different factor $f^{(G)}$

$$f_{1,2,3,4}^{(G)} = \frac{1}{2} \left( \frac{1}{\xi_{1}^\downarrow - \xi_{2}^\downarrow} + \frac{1}{\xi_{3}^\downarrow - \xi_{4}^\downarrow} \right). \quad (22)$$

A general feature of the continuous canonical transformation is that it derives the effective
Hamiltonians avoiding any singularities for the renormalized energies and interactions [7,8].

For instance, the effective retarded interaction between electrons in a coupled electron-
phonon system has been shown to be $-|M_{q}^{el-ph}|^2 \omega_q \left[ (\xi_{k+q} - \xi_{k})^2 + \omega_q^2 \right]^{-1}$ [3] instead of the
divergent Fröhlich result $|M_{q}^{el-ph}|^2 \omega_q \left[ (\xi_{k+q} - \xi_{k})^2 - \omega_q^2 \right]^{-1}$ [24] ($M_{q}^{el-ph}$ denotes the electron phonon coupling and $\omega_q, \xi_{k}$ refer to phonon and electron energies respectively).
A similar situation takes place in the DEX model studied here. For small values of $J_H S$ (as compared to the electron bandwidth) we obtain less divergent factor \((21)\) than it has been predicted from the standard canonical transformation \((22)\) found in the Refs \([19,20]\). For the limit of large $J_H S$ both factors \((21,22)\) asymptotically approach $f \sim -(J_H S)^{-1}$ and effectively $M^\sigma \sim 0, U \sim -J_H/2$.

In the limit $l \to \infty$, the exchange interaction \([6]\) is absent and then one can roughly estimate the magnon dispersion as

$$\omega_q = \frac{1}{N} \sum_k \left[ M_{k,k,q,q}^\uparrow n_k^\downarrow - M_{k,k,q,q}^\downarrow n_k^\uparrow \right].$$

Here the expectation value $n_k^\sigma = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle$ has a meaning of the Fermi-Dirac distribution function of the argument $\xi_k^\sigma (l = \infty)$. By inspecting the expressions \((21,22)\) one notices that the diagonal terms $f_{1,2,3=1,4=2}$ are in both cases identical, independently on magnitudes of $J_H$ and $S$. Effectively, the magnon spectrum becomes

$$\omega_q = \frac{J_H}{2N} \sum_k \left( n_k^\uparrow - n_k^\downarrow \right) + \frac{J_H^2 S}{2N} \sum_k \frac{n_k^\downarrow - n_{k+q}^\downarrow}{\xi_k^\downarrow - \xi_{k+q}^\downarrow}.$$  

Our lowest order estimation \((24)\) is thus in agreement with predictions based on the standard canonical transformation \([19,20]\) and other earlier studies of this model \([23,27]\) as well. The gapless Goldstone mode $\omega_{q=0} = 0$ (for arbitrary temperature and $J_H$) marks the spontaneous breaking of rotational symmetry.

**IV. SELFCONSISTENCY CORRECTIONS**

In this section we take into account the effect of the terms neglected by us so far in the equation \((10)\). We postulate that the effective Hamiltonian should be given in the form $H_0(l)$ \([1]\) with some small correction expressed there by $\delta H_0(l)$. Following other studies based on the flow equation method we consider effect of the higher order interactions by reducing them to normally ordered form. As can be seen below, $\delta H_0(l)$ would then be expressed by the fluctuations around the mean field values, which should be small.
i) Correction of the order $O(IU)$ arises from the commutator between $\eta$ and the electron electron interaction. It is easy to verify that this term can be expressed as follows

\[
O(IU) = \frac{1}{N}\sum_{k,q} \alpha_{k,q}(l) I_{k,q}(l) \sum_{k',p',p''} U_{k',p',p'',k''}(l) \delta_{k'+p',k''+p''} \\
\times a_q^\dagger \left( c_{p'}^\dagger c_{k''}^\dagger c_{k} \delta_{k-q, p''} - c_{k-q}^\dagger c_{p'}^\dagger c_{k''}^\dagger \delta_{k,k'} \right) + \text{h.c.} \\
= :O(IU): + \frac{1}{N}\sum_{k,q} a_q^\dagger c_{k-q} \sum_{k'} \left[ \alpha_{k',q}(l) I_{k',q}(l) U_{k',k-q,k'-q}(l) \left( n_{k'}^\downarrow - n_{k'}^\uparrow \right) \right] \\
- \alpha_{k,q}(l) I_{k,q}(l) \left( U_{k,k-q,k'-q,k}(l) n_{k'}^\downarrow - U_{k,k-q,k-k',l}(l) n_{k'}^\uparrow \right) \right] + \text{h.c.} \quad (25)
\]

ii) The other term $O(IM)$ comes from the commutator between $\eta$ and the magnon electron interaction. Its contribution to the flow equation is

\[
O(IM) = \frac{1}{N}\sum_{k,q} \alpha_{k,q}(l) I_{k,q}(l) \sum_{k',q',q''} \left[ \delta_{q,q'} M_{k',k',q',q''}(l) c_{k'}^\dagger c_{k''}^\dagger c_{q'}^\dagger c_{q''}^\dagger \\
- M_{k',k',q',q''}(l) c_{k'}^\dagger c_{q'}^\dagger c_{q''}^\dagger c_{k''}^\dagger a_q^\dagger a_q^\dagger + a_q^\dagger a_q^\dagger M_{k',k',q',q''}(l) c_{k'}^\dagger c_{k''}^\dagger a_{q'}^\dagger a_{q''}^\dagger + h.c. \right] \\
= :O(IM): + \frac{1}{N}\sum_{k,q} a_q^\dagger c_{k-q} \left\{ \alpha_{k,q}(l) I_{k,q}(l) \left[ \sum_{k'} \left( M_{k',k',q,q}(l) n_{k'}^\dagger \\
- M_{k',k',q,q}(l) n_{k'}^\dagger \right) + \sum_{q''} \left[ \left( 1 - n_{k-q}^\dagger \right) M_{k-q,k-q,q',q''}(l) a_{q'}^\dagger a_{q''}^\dagger + h.c. \right] \right] \right\} + \text{h.c.} \quad (26)
\]

We introduced here the expectation value for the magnon’s number operator $n_q = \langle a_q^\dagger a_q \rangle$, which can be approximately taken as the Bose-Einstein distribution function of the magnon energy $\omega_q$.

From now on, we put the both contributions (25,26) into the $\delta H_0(l)$ part of the Hamiltonian and neglect there the normally ordered parts : $O(IU) :, : O(IM) :$ which are supposed to be small. We neglect also a contribution to the flow equation which might arise from the commutator $[\eta, \delta H_0]$. This is the only simplification we need in order to close the set of flow equations for the Hamiltonian $H_0(l) + H_{int}(l)$. By inspecting the structure of expressions (25,26) we conclude that the flow equations (12-17) remain unchanged. The only quantity
affected directly is the exchange coupling constant $I_{k,q}(l)$. The revised flow equation (11) is now given by

$$
\frac{dI_{k,q}(l)}{dl} = -\alpha_{k,q}^2(l)I_{k,q}(l) + \alpha_{k,q}(l)I_{k,q}(l) \left\{ \frac{1}{N} \sum_{k'} \left[ (U_{k,k',k,k'}(l) - M_{k,k',k,k'}^+(l)) n_{k'}^+ \right] - \frac{1}{N} \sum_{q} n_q \left[ (M_{k-k-k,q,q}^+(l) - M_{k,k,q,q}^+(l)) \right] + \frac{1}{N} \sum_{k'} \left[ (1 - n_{k-k}' + n_{q}'(l) M_{k-k-k,q,q}^+(l) \alpha_{k,q}(l)I_{k,q}(l) \cdot \right] \cdot (27)
$$

We studied numerically the system of coupled flow equations (12-15,27) solving them self-consistently via the Runge Kutta algorithm. Since the model parameters such as $U_{k,q,p,k+q-p}$ and $M_{k,q,p,k+q-p}$ depend on three momenta it is a rather cumbersome task to study the 3 or even 2 dimensional systems. For a demonstration we therefore used the one dimensional tight binding lattice with its initial dispersion $\varepsilon_k(l = 0) = -2t \cos ka$. From now on, we set the lattice constant $a = 1$ and choose the initial bandwidth as a unit $W = 4t \equiv 1$ (flow parameter $l$ will be expressed in units of $W^{-2}$).

We discretized the first Brillouin zone with a mesh of 200 equally distant points. Starting from the initial conditions (8) we computed iteratively the renormalized model parameters using a following scheme $y(l + \delta l) = y(l) + y'(l)\delta l$ where $y'(l) \equiv dy(l)/dl$ and it is given by one of the flow equations (12-15,27) for a corresponding parameter $y$. Increment of the flow parameter was taken $\delta l = 0.0001$ for $l \leq 0.1$ and $\delta l = 0.001$ for $l \in (0.1; 1.0)$.

Figure 1 shows how the model parameters evolve with an increasing $l$. Practically, already from $l = 0.3$ these quantities start to saturate at their asymptotic values. The exchange interaction disappears very fast, whereas the magnon - electron interaction is reduced roughly 10 times. There occurs some renormalization of $\varepsilon_k$ electron energies and a simultaneous induction of a relatively strong electron – electron attractive interactions.
FIG. 1. Evolution of the DEX model parameters with respect to a varying flow parameter \( l \) at \( T = 0 \) and hole concentration 0.3. Individual lines correspond to the following quantities: 

\[ I \equiv \frac{1}{N^2} \sum_{k,q} |I_{k,q}|^2, \quad \varepsilon \equiv \frac{1}{N} \sum_k (\varepsilon_k)^2, \quad U \equiv \frac{1}{N^2} \sum_{k,p,q} |U_{k,p,q,k+p,q}|^2 \quad \text{and} \quad M \equiv \frac{1}{N^2} \sum_{k,p,q} |M_{k,p,q,k+p,q}|^2. \]

FIG. 2. Plot of the normalized exchange coupling \( I_{kq}(l = 1)/I_{kq}(l = 0) \). This interaction is weak enough to be considered as negligible.
Figure 2 illustrates what is left of the exchange interaction at \( l = 1 \). The highest values of \( I_{k,q} \) are \( 7 \times 10^{-5} \) of the initial interaction \( J_H \sqrt{S/2} \). Such small magnitude is in our opinion negligible and thereof we represent below the effective model parameters (formally corresponding to \( l = \infty \)) through their values obtained at \( l = 1 \).

Let us next have a brief look on the electron part. In figure 3 we plot the dispersion for spin \( \sigma = \downarrow \) electrons obtained from the selfconsistent solution of the flow equation (12). Effective bandwidth becomes of the order \( \sim 0.83 \) of the initial bare bandwidth \( W \). This renormalization is weaker than a result of the standard canonical transformation \([19,20]\), which gave the scaling factor \( \sim 0.64 \). As concerns the effective mass we notice a similar tendency. The whole band of \( \sigma = \downarrow \) electrons drifts away from the partly occupied band of \( \sigma = \uparrow \) electrons increasing the gap between them which initially was \( J_H S \). The flow equation method gives a somewhat smaller shift than the standard canonical transformation.

![Dispersion for spin \( \sigma = \downarrow \) electrons](image)

**FIG. 3.** The effective dispersion for spin \( \sigma = \downarrow \) electrons obtained from a selfconsistent solution of the flow equations (solid line) and via the standard single step transformation (dashed line). The dotted curve shows the initial bare dispersion \( \varepsilon_k = -2t \cos ka \).

Figure 4 shows a strength of the induced electron – electron interaction for the BCS channel \( U_{k,-k,-q,q} \) (scattering between the electron pairs of the total zero momentum). This interaction is again weaker by almost 30 % from the corresponding magnitude determined by the standard transformation. It should be stressed here that electron – electron interactions
may eventually play important role in a low energy physics of the DEX model only when hole concentration $1 - n$ is close to zero. Otherwise, the scattering processes between particles originating from so much separated ($\sim J_H S$) electron bands would not become efficient.

FIG. 4. The effective interaction between electrons in the zero momentum BCS channel, i.e. $U_{k,-k,-q,q}c_{k\downarrow}^\dagger c_{-k\uparrow}c_{-q\uparrow}c_{q\downarrow}$. Other elements of the potential $U_{k,p,q,k+p-q}$ take on average the same values as shown in this picture (around $-0.8$).

If the initial Hund's coupling $J_H$ is large and hole doping is not close to zero then the low energy physics of the effective Hamiltonian $H(l = \infty)$ is mainly determined from the electron–magnon interaction. This interaction is characterized by two coupling constants $M_{k,p,q,k-p+q}^\sigma$ which, according to our numerical estimation, can vary between $-0.5$ and $0.5$ depending on the momenta $q, k, p$ and only slightly on temperature $T$ and concentration $n$. In general, in this method we find that absolute values of both coupling constants $M^\sigma$ become reduced by 10 to 20% as compared to the result of the standard transformation (given in equation (19) with the $f(G)$ factor (22)). Figure 5 shows this effect on the example of the diagonal part $M_{k,k,q,q}^\uparrow$ (notice, that in the approximate solution discussed in section III there was no difference between both methods for such diagonal elements).
FIG. 5. Potential of the electron – magnon interaction $M^\uparrow_{k,k,q,q}$ obtained from a selfconsistent solution of the flow equations (solid lines) and from the standard canonical transformation (dashed curves). We used three representative values for the momentum $q$ as marked on a right corner of the figure.

A natural expectation is that reduction of the electron - magnon interaction would in a consequence affect such quantities like magnon spectrum, the life-time of these quasiparticles and finally also the Curie critical temperature. It is not a scope of this paper to study all these effects (we mainly intend to present this new technique for a derivation of the effective Hamiltonian). To get some insight we present below a rough estimation of the magnon dispersion based on the lowest order formula (23). Higher order corrections are straightforward to carry out but we believe they would not alter anything in this context.

In the lowest order perturbative determination of the magnon dispersion $\omega_q$ we simply need only the diagonal parts $M^\sigma_{k,k,q,q}$ and at low temperatures main contribution comes from $\sigma = \uparrow$. In the long wavelength limit $q \to 0$ for $\omega_q$ one gets a parabolic momentum dependence with the spin stiffness coefficient $D_s = \lim_{q \to 0} \omega_q / q^2$. Using the standard expression (24) Furukawa [26] gave an explicit formula for $D_s$ at low $T$ and studied $D_s$ with respect to $J_H$ and the hole concentration $p = 1 - n$ (where $n = \sum_{k,\sigma} < c_{k\sigma}^\dagger c_{k\sigma}>$). For a comparison we show in the figures 6 and 7 our results.
FIG. 6. Spin stiffness $\tilde{D}_s \equiv 2SD_s/t$ as a function of the inverse Hund’s coupling for $T = 0$ and hole concentration 0.3. Solid line shows a result obtained from the flow equation method and the dashed one refers a standard estimation based on equation (24).

FIG. 7. Spin stiffness $\tilde{D}_s$ as a function of hole concentration for $J_H/W = 2, T = 0$ obtained from the flow equation method (solid curve) and the single step transformation (dashed line).
Due to a discussed above reduction of the electron – magnon coupling (see figure 3) we notice a partial softening of the spin stiffness in a whole regime of carrier concentration. Such a softening takes place mostly for the strong Hunds coupling. Going towards the limit of small $J_H$ this effect becomes less pronounced. In particular, for $J_H = 2W$ and hole concentration $p = 0.3$ our result for $D_s$ is almost 20% smaller as compared to the standard result reported by Furukawa [26].

This tendency for a softening of the spin stiffness (especially in a limit of large $J_H$) agrees qualitatively with the results reported recently by Shannon and Chubukov [4] who introduced a novel large $S$ expansion scheme for systems with strong Hund’s coupling. Authors showed that quantum effects caused a relative softening of spin-wave modes at the zone center. There is a rich literature where authors report differences between the Heisenberg cosine dispersion (for $\omega_q$) and the actual dispersion found from the calculations for DEX model [22,26,28]. In those papers a relative flattening of the dispersion $\omega_q$ near the zone boundaries has been found. Our results follow closely the same behavior.

At the end of this section we would like to make an effort to analyze in more detail the effect of some neglected terms: $O(IU)$: and $O(IM):$. As an illustration, let us consider one of possible contributions to $\delta H_0(l)$

$$\delta H_0^{(1)}(l) = \frac{1}{N\sqrt{N}} \sum_{q,k,p,p',p''} V_{q,k,p',p''}(l) : a_{q-k-q}^\dagger c_{p'}^\dagger C_{p''}^\dagger c_{k+p'-p''} :$$

(28)

taken from: $O(IU)$: [25]. Its initial ($l = 0$) amplitude is of course $V_{q,k,p',p''}(l = 0) = 0$. The flow equation corresponding to this potential is given by

$$\frac{dV_{q,k,p',p''}(l)}{dl} = -\alpha_{k,q}(l)I_{k,q}(l)U_{k,p',p''}c_{k+p'-p''}(l) .$$

(29)

We checked numerically that the potential $V$ of the interaction (28) is negative. On average, its value is $1/N^4 \sum_{k,q,p',p''} V_{q,k,p',p''} \simeq -0.4$ which is close to strength of the electron – magnon interactions $< M^\sigma >$. To be specific we show in figure 8 this potential in two channels: $V_{0-k,-k,q}(l) a_{0-k-q}^\dagger c_{-k-q}^\dagger c_{-k}^\dagger c_{q}^\dagger$ (top picture) and $V_{q,k,-k,-k}(l) a_{q-k-q}^\dagger c_{-k-q}^\dagger c_{-k}^\dagger c_{k}^\dagger$ (bottom picture).
Such many body interactions would however be not efficient at low temperatures because they engage electrons from vastly distant bands (similarly as the electron–electron inter-

FIG. 8. Potential of the many body interaction given in the equation (28) at $T = 0$ and hole concentration 0.3
action $U$). Moreover, we have only the normal ordered part of this interaction entering to
the Hamiltonian, and that should be small. The mean field value of this type interactions
were already included by us in the flow equation for $I_{k,q}$ (27).

Having interactions shown in (28), one can induce from $[\eta(l), \delta H_0^{(1)}(l)]$ next generation
of higher order interactions, like for example $c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger c_{3\uparrow} c_{4\uparrow}^\dagger a_5^\dagger a_6$. They can be found in the
standard canonical transformation as well (see $H'_4$ in the Ref. [20]). However let us repeat
again, that in our case we get only the normal ordered forms of all such higher order inter-
actions. So, hopefully, their influence on a physics of the effective Hamiltonian should be
relatively negligible.

V. CONCLUSIONS

In summary, we formulated continuous canonical transformation for the double exchange
model, eliminating from the initial Hamiltonian the exchange interaction term responsible
for a violation of magnon number. Thus, in a limit $l \rightarrow \infty$, true magnons are obtained.
Parameters of the effective Hamiltonian are determined via the set of the flow equations
(12-15) and (27). Structure of the resulting Hamiltonian (6) is simple but the effective
model parameters are computed selfconsistently taking into account effect of the higher
order interactions (what is not possible in the standard single step transformation). These
feedback effects are discussed by us on example of the magnon dispersion. We find a partial
softening of the spin stiffness in a whole regime of hole concentration.

Further studies are needed to solve the flow equations for a realistic 3D version of the
DEX model. Another important issue not studied here is to extend the procedure to capture
the damping effects for magnons and electrons. As discussed earlier in the context of different
models [11,29] one should study then the flow not only of the whole Hamiltonian $H(l)$ but
also for the particular operators like $a_q^{(l)}$. Such an investigation for the DEX model is in
progress and the results will be reported elsewhere.
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