Vol. 32 (2001) *ACTA PHYSICA POLONICA B* No 10 Special Issue

THE FLOW EQUATION STUDY OF FERROMAGNETISM IN THE DOUBLE EXCHANGE MODEL*

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(Received June 21, 2001)

The Double EXchange (DEX) model for ferromagnetism is studied by means of the flow equation method. The initial Hamiltonian is lead through a set of the infinitesimal unitary transformations which eliminate from it the part responsible for violation of the magnon number. Basic properties of the effective Hamiltonian are discussed.

PACS numbers: 71.70.Gm, 75.10.–b, 75.30.Et

Colossal magnetoresistance which has been observed in the doped manganese oxides $R_{1-x}A_x\mathrm{MnO}_3$ (where *e.g.* R =La, Sr, Nd and A =Ca, Sr, Ba) near their transition to ferromagnetic state is often attributed to the double exchange mechanism [1–3]. It is the Kondo type interaction between conduction electrons and spins of the localized Mn ions ($-J_{\rm H}\sum_{i,\alpha,\beta}\vec{S}_i c^{\dagger}_{i,\alpha}\vec{\sigma}_{\alpha\beta}c_{i,\beta}$, where here $J_{\rm H}$ denotes the Hunds coupling) which leads to maximization of electron kinetic energy when spins (of immobile Mn ions) are ordered ferromagnetically. Despite the intensive studies of this model ranging from the standard mean field [4,5], the QMC simulations [6] and the dynamical mean field approach [3] there are still some unclear issues like for instance estimation of transition temperature T_c into ferromagnetic phase, determination of magnon dispersion, life time effects for magnons *etc.* Here we would like to present some results obtained for the DEX model with a novel approach of the continuous canonical transformation which is known in the literature as *the flow equation method* [7, 8].

We start from introducing the Holstein boson representation for the localized spin operators $\vec{S}$ which, at sufficiently low temperatures, are given

* Presented at the XII School of Modern Physics on Phase Transitions and Critical Phenomena, Lądek Zdrój, Poland, June 21–24, 2001.

by $S_i^- \simeq a_i^\dagger \sqrt{2S}$, $S_i^+ = (S_i^-)^\dagger$, $S_i^z = S - a_i^\dagger a_i$. In terms of the magnon operators $a_i^{(\dagger)}$ one can express the DEX Hamiltonian as

$$\begin{aligned} H \;=\; & \sum_{\boldsymbol{k}} \left[\left(\xi_{\boldsymbol{k}} - \frac{J_{\mathrm{H}} S}{2} \right) c_{\boldsymbol{k}\uparrow}^\dagger c_{\boldsymbol{k}\uparrow} + \left(\xi_{\boldsymbol{k}} + \frac{J_{\mathrm{H}} S}{2} \right) c_{\boldsymbol{k}\downarrow}^\dagger c_{\boldsymbol{k}\downarrow} \right] \\ & + \frac{J_{\mathrm{H}}}{2N} \sum_{\boldsymbol{q},\boldsymbol{p},\boldsymbol{k}} a_{\boldsymbol{p}+\boldsymbol{q}}^\dagger a_{\boldsymbol{p}} \left(c_{\boldsymbol{k}-\boldsymbol{q}\uparrow}^\dagger c_{\boldsymbol{k}\uparrow} - c_{\boldsymbol{k}-\boldsymbol{q}\downarrow}^\dagger c_{\boldsymbol{k}\downarrow} \right) \\ & - J_{\mathrm{H}} \sqrt{\frac{S}{2N}} \sum_{\boldsymbol{q},\boldsymbol{k}} \left(a_{\boldsymbol{q}}^\dagger c_{\boldsymbol{k}-\boldsymbol{q}\uparrow}^\dagger c_{\boldsymbol{k}\downarrow} + \mathrm{h.c.} \right) , \end{aligned} \tag{1}$$

where $\xi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - \mu$. The first term describes kinetic contribution of the split electron band, the second one refers to density–density interaction between electrons and magnons and the last term represents interaction which violates number of magnons. The standard canonical transformation known from literature [9, 10] is able to eliminate such nonconserving (in magnon number) part

$$V \equiv -J_{\mathrm{H}} \sqrt{\frac{S}{2N}} \sum_{\boldsymbol{q},\boldsymbol{k}} \left(a_{\boldsymbol{q}}^\dagger c_{\boldsymbol{k}-\boldsymbol{q}\uparrow}^\dagger c_{\boldsymbol{k}\downarrow} + \mathrm{h.c.} \right) \tag{2}$$

but in turn it generates many other types of interactions. Unlike [9, 10] we want to renormalize (1) via the sequence of canonical transformations $H(l) = U^\dagger(l) H U(l)$ such that the Hamiltonian structure shall be kept as simple as possible. In the limit $l \to \infty$ the part (2) would disappear. A continuous way of transforming the Hamiltonian gives us more control on preserving the needed structure of that operator.

In practice, it is not necessary to specify an explicit form of the unitary operator $U(l)$, but one can instead choose the generating operator η (which is related to $U(l)$ through $\eta \equiv dU^\dagger(l)/dl)U(l))$. The generating operator η governs a *flow* of the Hamiltonian via $dH(l)/dl = [\eta, H]$ (and similar flow equation can be written for any other operator like $c_{i,\sigma}^{(\dagger)}(l)$, $a_i^{(\dagger)}(l)$). Wegner [7] has proved that with $\eta = [H, V]$ one can project out the perturbation $V(l)$ in the limit $l \to \infty$ unless the degenerate states are encountered.

In a separate paper one of us [11] gave a detailed derivation of the flow equations for parameters of the effective Hamiltonian of this model. To summarize we present below the final form of the DEX Hamiltonian

$$H(l=\infty) \;=\; \sum_{\boldsymbol{k}} \left[\left(\xi_{\boldsymbol{k}} - \frac{J_{\mathrm{H}} S}{2} \right) c_{\boldsymbol{k}\uparrow}^\dagger c_{\boldsymbol{k}\uparrow} + \left(\xi_{\boldsymbol{k}} + \Delta\varepsilon_{\boldsymbol{k}}^{\downarrow} + \frac{J_{\mathrm{H}} S}{2} \right) c_{\boldsymbol{k}\downarrow}^\dagger c_{\boldsymbol{k}\downarrow} \right]$$

$$+\frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\boldsymbol{q}'}\delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{k}'+\boldsymbol{q}'}\Big[U_{\boldsymbol{k},\boldsymbol{q},\boldsymbol{q}',\boldsymbol{k}'}c^\dagger_{\boldsymbol{k}\downarrow}c^\dagger_{\boldsymbol{q}\uparrow}c_{\boldsymbol{q}'\uparrow}c_{\boldsymbol{k}'\downarrow}$$
$$+\left(M^\uparrow_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\boldsymbol{q}'}c^\dagger_{\boldsymbol{k}\uparrow}c_{\boldsymbol{k}'\uparrow}-M^\downarrow_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\boldsymbol{q}'}c^\dagger_{\boldsymbol{k}\downarrow}c_{\boldsymbol{k}'\downarrow}\right)a^\dagger_{\boldsymbol{q}}a_{\boldsymbol{q}'}\Big]. \qquad (3)$$

One notices renormalization of the kinetic energy of $\sigma=\downarrow$ electrons ($\Delta\varepsilon^\downarrow_{\boldsymbol{k}}$), modification of the initial density–density interaction between electrons and magnons (now it is labelled with three momenta and depends on spin of electrons) and, finally also generation of the effective interaction between opposite spin electrons. To characterize quantitatively effect of renormalizations we solved numerically the set of coupled flow equations using one-dimensional tight binding dispersion for electrons and some realistic values for the model parameters. We chose the initial Hunds coupling $J_{\rm H}=2W$ (W stands for electron bandwidth) and set temperature $T=0$.

In figure 1 we show the resulting density of states $\rho(\omega)=\sum_{\boldsymbol{k},\sigma}\delta\left(\omega-\varepsilon^\sigma_{\boldsymbol{k}}\right)$. Electronic spectrum consists of two subbands which are roughly split by $J_{\rm H}S$. Due to the correction $\Delta\varepsilon^\downarrow_{\boldsymbol{k}}$ the upper band becomes narrowed and pulled down. This effect can be important if electron concentration approaches half-filling $n=1$.

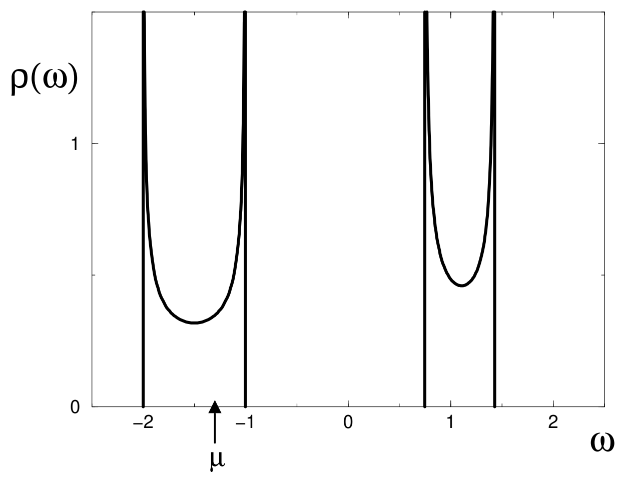

Fig. 1. Density of states of the DEX model for $T=0$ and hole concentration $x=0.25$. Electron spectrum consists of the partly filled lower band (of spin $\sigma=\uparrow$ species) partly and the upper one which is empty.

The other quantity which is modified in a course of continuous canonical transformation is the strength of magnon electron interaction. This effect is thoroughly discussed in the quoted paper [11]. Let us remark here that such interaction affects the excitation magnon spectrum. In the lowest order estimation (the bubble diagram) one obtains for magnon energy

$\omega_{\boldsymbol{q}} = 1/N \sum_{\boldsymbol{k}} \left[M^{\uparrow}_{\boldsymbol{k},\boldsymbol{k},\boldsymbol{q},\boldsymbol{q}} n^{\uparrow}_{\boldsymbol{k}} - M^{\downarrow}_{\boldsymbol{k},\boldsymbol{k},\boldsymbol{q},\boldsymbol{q}} n^{\downarrow}_{\boldsymbol{k}} \right]$. From the numerical investigation we found considerable softening of the magnon stiffness $\lim_{\boldsymbol{q}\to 0} \omega_{\boldsymbol{q}}/q^2$ as compared to predictions of the standard canonical transformation [9, 10]. This result (being sensitive to both $J_{\rm H}$ and hole concentration $x = 1 - n$) seems to agree with recent results by Shannon and Chubukov [12] who used the modified large S expansion method.

Finally, we present in figure 2 strength of the induced attraction between electrons of opposite spins. Effect of such interactions would perhaps be not much important deep in the ferromagnetic phase (where only $\sigma = \uparrow$ exist) but with an increasing temperature and/or approaching the electron concentration $n \sim 1$ its effectiveness would increase.

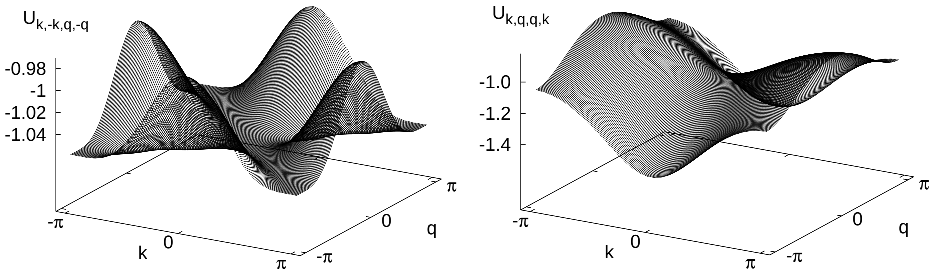

Fig. 2. The interaction generated between electrons in the BCS zero momentum channel (left figure) and density channel (right figure).

In conclusion we reported the results of the flow equation method applied to the DEX model. Method enables us to obtain true magnons (their concentration being conserved quantity) while rescaling other parameters of the model Hamiltonian. Future studies are needed to determine the correlation functions which would help to determine *e.g.* the transition temperature T_c. Such calculations are in progress and the results will be published elsewhere.

This work was supported by the Polish State Committee for Scientific Research under grant No 2P03B 106 18.

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