Paramagnetic-ferromagnetic transition in a double-exchange model

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We study paramagnetic-ferromagnetic transition due to exchange interaction between classical localized magnetic moments and conduction electrons. We formulate the Dynamical Mean Field Approximation equations for arbitrary electron dispersion law, concentration and relation between exchange coupling and the electron band width. Solving these equations we find explicit formula for the transition temperature $T_c$. We present the results of calculations of the $T_c$ for the semi-circular electron density of states.

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I. INTRODUCTION

The double-exchange (DE) model [1–3] is one of the basic ones in the theory of magnetism. Magnetic ordering appears in this model due to exchange coupling between the core spins and the conduction electrons. The Hamiltonian of the model is

\begin{equation}
H = \sum_{n\alpha} t_{n-n'} c_{n\alpha}^\dagger c_{n'\alpha} - J \sum_{n\alpha\beta} S_n \cdot \sigma_{\alpha\beta} c_{n\alpha}^\dagger c_{n\beta},
\end{equation}

where $c$ and $c^\dagger$ are the electrons annihilation and creation operators, $S_n$ is the operator of a core spin, $t_{n-n'}$ is the electron hopping, $J$ is the exchange coupling between a core spin and $n$ electrons, $\sigma$ is the vector of the Pauli matrices, and $\alpha, \beta$ are spin indices.

The model (the core spins being treated as classical vectors) began to be studied several decades ago [1–3]. Because of a recent general interest in manganites, it reappeared in the focus of attention (see reviews [4–7] and references therein). In particular, application of the Dynamical Mean Field Approximation (DMFA) [8] substantially advanced our understanding of the properties of the DE model [9,10]. Most of the papers dealing with the model, starting from classical paper by De Gennes [3], considered the DE Hamiltonian with infinite exchange (and with the addition of the antiferromagnetic superexchange, which is crucial for the explanation of magnetic properties of manganites). However lately many properties of the model for arbitrary strength of the exchange were analyzed [11].

In this paper we calculate the temperature of a paramagnetic-ferromagnetic transition $T_c$ in a double-exchange model for arbitrary electron dispersion law, concentration and relation between the exchange coupling and the electron band width by formulating and solving the DMFA equations. We treat the core spins as classical vectors.

II. DMFA EQUATIONS AND $T_C$

Spins being considered as classical vectors $S_n = m_n$ (with the normalization $|m|^2 = 1$), the problem becomes a single electron one. The DE Hamiltonian in a single electron representation can be presented as

\begin{equation}
H_{nn'} = t_{n-n'} - J m_n \cdot \sigma \delta_{nn'}.
\end{equation}

Let us introduce Green’s function

\begin{equation}
\hat{G}(E) = (E - H)^{-1}
\end{equation}

and local Green’s function

\begin{equation}
\hat{G}_{\text{loc}}(E) = \left\langle \hat{G}_{nn}(E) \right\rangle.
\end{equation}

In the last Equation, the averaging is with respect to random configurations of the core spins. In the framework of the DMFA approach to the problem (see [8,10] and references therein) the local Green’s function is expressed through the the local self-energy $\hat{\Sigma}$ by the equation

\begin{equation}
\hat{G}_{\text{loc}}(E) = g_0 \left( E - \hat{\Sigma}(E) \right),
\end{equation}

where

\begin{equation}
g_0(E) = \frac{1}{N} \sum_k (E - t_k)^{-1}
\end{equation}

is the bare (in the absence of the exchange interaction) local Green’s function. The self-energy satisfies equation

\begin{equation}
\hat{G}_{\text{loc}}(E) = \left\langle \frac{1}{G_{\text{loc}}^{-1}(E) + \hat{\Sigma}(E) + J m \cdot \hat{\sigma}} \right\rangle,
\end{equation}

where $\langle X(m) \rangle \equiv \int X(m) P(m)$, and $P(m)$ is a probability of a given spin orientation (one-site probability). The quantities $\hat{G}$ and $\hat{\Sigma}$ are $2 \times 2$ matrices in spin space.
The difference between Eq. (7) and similar equation appearing in the Coherent Potential Approximation [12], is due to the fact that in our problem the disorder is annealed (and not quenched). That is the probability of a given (random) core spin configuration is determined by the energy of electron subsystem interacting with this configuration.

To understand the DMFA assumption allowing to find the probability \( P(\mathbf{m}) \) self-consistently with the solution of Eq. (7), notice that Eq. (7) reduces the problem of electron scattering by many spins, to scattering by a single spin with the effective potential \( V = -J\mathbf{m}\sigma - \Sigma \). The spin is embedded in an effective medium, described by the Hamiltonian \( t_k + \Sigma \), and, hence, by the local Green’s function \( \bar{G}_{\text{loc}} \). Consider the change in the number of electron states in such system due to a single spin. We get [12,13]

\[
\Delta D(E, \mathbf{m}) = -\frac{1}{\pi} \text{Im} \ln \det \left[ 1 + \left( \mathbf{Jm}\sigma + \Sigma \right) \bar{G}_{\text{loc}} \right], \tag{8}
\]

where the argument of both \( G_{\text{loc}} \) and \( \Sigma \) is \( E + i0 \). So the change in thermodynamic potential is [14,11,15]

\[
\Delta \Omega(\mathbf{m}) = \int f(E) \Delta D(E, \mathbf{m}) dE, \tag{9}
\]

where \( f(E) \) is the Fermi function. The DMFA approximation for the one-site probability \( P(\mathbf{m}) \) is:

\[
P(\mathbf{m}) \propto \exp \left[ -\beta \Delta \Omega(\mathbf{m}) \right]. \tag{10}
\]

Eqs. (7) and (10) are the system of non-linear (integral) equations. However, the system is grossly simplified in paramagnetic (PM) phase, where the macroscopic magnetization \( \mathbf{M} = 0 \). In this case \( P(\mathbf{m}) = \text{const.} \), the averaging in Eq. (7) can be performed explicitly, and we obtain

\[
g(E) = \frac{1}{2} \sum_{\pm} \frac{1}{g^{-1}(E) + \Sigma(E) \pm J}, \tag{11}
\]

where \( \Sigma = \Sigma \hat{1}, \hat{G} = g\hat{1} = g_0(E - \Sigma)\hat{1}, \) where \( \hat{1} \) is a unity matrix.

In the ferromagnetic (FM) phase near the Curie temperature, Eqs. (7) and (10) can be linearized [9,11] with respect to \( \mathbf{M} \). Thus we reduce the DMFA equations to a traditional MF equation [16]

\[
P(\mathbf{m}) \propto \exp \left[ -3\beta T_c \mathbf{M} \cdot \mathbf{m} \right]. \tag{12}
\]

The parameter \( T_c \) is formally introduced as a coefficient in the expansion of \( \Delta \Omega(\mathbf{m}) \) with respect to \( \mathbf{M} \). Non-trivial solution of the MF equation

\[
\mathbf{M} = \langle \mathbf{m} \rangle \tag{13}
\]

can exist only for \( T < T_c \), hence \( T_c \) is the ferromagnetic transition temperature. In all cases \( T_c \) turns out to be much less the chemical potential, so we can consider electron gas as degenerate. In this case

\[
\int_{-\infty}^{\infty} f(E) \ldots dE \equiv \int_{-\infty}^{\mu} \ldots dE, \tag{14}
\]

where the chemical potential (in paramagnetic phase) is found from the equation

\[
n = -\frac{2}{\pi} \int_{-\infty}^{\mu} \text{Im} \ g \ dE, \tag{15}
\]

and \( n \) is the number of electrons per site.

For the \( T_c \), after straightforward, though lengthy algebra, we obtain

\[
T_c = \frac{2J^2}{3\pi} \int_{-\mu}^{\mu} \text{Im} \left[ \frac{g}{g^2 + 2J^2 g^2 - \frac{2J^2 g^2}{4}} \right] dE, \tag{16}
\]

where \( \Sigma \) and \( g \) are determined by the properties of the system in the PM phase; they are the solutions of Eqs. (5) and (11); \( g' = \frac{dg_{\nu}(\epsilon)}{d\epsilon} |_{\epsilon = E - \Sigma} \). Eq. (16) is the main result of our paper.

In the case of weak exchange \( J \rightarrow 0 \) Eq. (16) takes the form

\[
T_c = \frac{2J^2}{3} \left[ N_0(\mu) - \frac{1}{\pi} \int_{-\infty}^{\mu} \text{Im} \ g_{\nu}(E) \right] dE. \tag{17}
\]

In fact, this equation is the MF approximation [16] for the RKKY Hamiltonian [17], to which the original Hamiltonian (1) can be reduced in the case \( J \ll W \).

In the opposite case \( J \rightarrow \infty \) we have to consider only one spin sub-band. (Because of the symmetry of the problem with respect to transformation \( n \rightarrow 2 - n \), everywhere further on we consider only the case \( n \leq 1 \).

After we shift \( E, \Sigma \) and \( \mu \) by \( J \), we obtain

\[
T_c = \frac{2}{\pi} \int_{-\infty}^{\mu} \text{Im} \left[ \frac{g' + g^2}{g' - 2g^2} \right] dE, \tag{18}
\]

where \( g \) is found from the equation

\[
g(E) = \frac{1}{2} \frac{1}{g^{-1}(E) + \Sigma(E)}. \tag{19}
\]

### III. \( T_c \) FOR SEMI-CIRCULAR DOS

Let us apply Eq. (16) to the case of semi-circular (SC) bare density of states (DOS)

\[
N_0(\epsilon) = \frac{2}{W} \sqrt{\left( \frac{\epsilon}{W} \right)^2 - 1}. \tag{20}
\]

Then
\[ g_0(E) = \int \frac{N_0(\varepsilon) d\varepsilon}{E - \varepsilon} = \frac{2}{W} \left[ \frac{E}{W} - \sqrt{\left( \frac{E}{W} \right)^2 - 1} \right]. \] (21)

From Eq. (5) follows
\[ \Sigma = E - W^2 g/4 - g^{-1}, \] (22)
and Eq. (11) can be written as
\[ g = \frac{1}{2} \sum_{(\pm)} \frac{1}{E - W^2 g/4 \pm J}. \] (23)

Eq. (16) takes the form
\[ T_c = \frac{J^2 W^2}{6\pi} \int_{-\infty}^{\mu} \text{Im} \left[ \frac{g^2}{(E - \frac{W^2 g}{4}) (E - \frac{W^2 g}{2}) - \frac{J^2 W^2}{6} g^2} \right] dE. \] (24)

In the case of weak exchange \( J/W \ll n^{1/3} \), we obtain
\[ T_c = \frac{4J^2}{3\pi^2 W} (4y^2 - 1) \sqrt{1 - y^2}, \] (25)
where
\[ n = n_0(y) \equiv 1 + \frac{2}{\pi} \left( \sin^{-1} y + y \sqrt{1 - y^2} \right). \] (26)

In the case of strong exchange \( J/W \gg n^{1/3} \), Eq. (18) takes the form \[ 10,15 \]
\[ T_c = \frac{W^2}{6\pi} \int_{-\infty}^{\mu} \text{Im} \left[ \frac{g^2}{1 - \frac{W^2 g^2}{6}} \right] dE \]
\[ = \frac{W \sqrt{2}}{4\pi} \left[ \sqrt{1 - y^2} - \frac{1}{\sqrt{3}} \tan^{-1} \sqrt{3(1 - y^2)} \right], \] (27)
where \( n = n_0(y)/2 \). If, in addition, \( n \ll 1 \), we obtain
\[ T_c = \frac{3}{4\sqrt{2}} W n \approx 0.53 \, W x. \] (28)

Notice, that virtual crystal approximation (for \( J \to \infty \)) [3] gives
\[ T_c = \frac{2}{15} W x \approx 0.13 \, W x, \] (29)
thus being imprecise by a factor of 4.

For arbitrary exchange, the integral in Eq. (24) can be calculated only numerically. The results of such calculation are presented on FIG. 1.

![Graph](image_url)

**FIG. 1.** \( T_c \) as a function of electron concentration \( n \) for different relative strengths of the exchange: \( J/W = 0.25 \) (dotted line), \( J/W = 1 \) (dash-dotted line), \( J/W = 2 \) (dashed line), and \( J/W = 20 \) (solid line).

**IV. NONFERROMAGNETISM**

Note that our main result (equation for the \( T_c \)) indicates it’s own limits of validity. In part of the \( J/W - n \) plane, Eq. (24) gives \( T_c < 0 \). Negative value of \( T_c \) means, that at any temperature, including \( T = 0 \), the paramagnetic phase is stable with respect to appearance of small spontaneous magnetic moment, and strongly suggests that the ground state in this part of the phase plane is nonferromagnetic [18]. The mechanisms leading to the destruction of ferromagnetism can be easily understood in the extreme cases of weak and strong exchange.

It is well known, that for \( J \to 0 \) the DE Hamiltonian can be reduced to the RKKY Hamiltonian (see review [17] and references to the original papers therein)
\[ H_{RKKY} = \sum_{nn'} I_{nn'} \mathbf{m}_n \cdot \mathbf{m}_{n'}. \] (30)

Thus weak exchange between the electrons and the core spins generates effective long-range and sign oscillating effective exchange interaction between the core spins.

In the opposite case \( J \to \infty \), we can reduce the DE Hamiltonian (2) to effective (classic) \( t - J \) model (see review [19] and references therein). To do that, first diagonalize the exchange part of the DE Hamiltonian by choosing local spin quantization axis on each site in the direction of \( \mathbf{m} \), the latter being determined by polar angle \( \theta \) and azimuthal angle \( \phi \). In this representation the Hamiltonian is
\[ H_{nn'} = -J \sigma_+ \delta_{nn'} + t_{nn'} \begin{pmatrix} a_{nn'} & b_{nn'} \\ b_{n'n}^* & a_{n'n} \end{pmatrix}, \] (31)
where
\[ a_{nn'} = \cos \frac{\theta_n}{2} \cos \frac{\theta_n'}{2} + \sin \frac{\theta_n}{2} \sin \frac{\theta_n'}{2} e^{i(\phi_n' - \phi_n)} \]
\[ b_{nn'} = \sin \frac{\theta_n}{2} \cos \frac{\theta_n'}{2} e^{-i\phi_n} - \cos \frac{\theta_n}{2} \sin \frac{\theta_n'}{2} e^{-i\phi_n'}. \] (32)
The next step is to apply a canonical transformation
\[ H \rightarrow \tilde{H} = e^S H e^{-S} = H + [S, H] + \frac{1}{2} [S[S, H]] + \ldots \] (33)
which excludes all band-to-band transitions. This can be achieved if we chose the operator \( S \) in the form
\[ S_{nn'} = -\frac{t_{nn'}}{2J} \begin{pmatrix} a_{nn'} & b_{nn'} \\ b_{n'n}^* & a_{n'n} \end{pmatrix}. \] (34)
We have
\[ [S, H^{ex}]_{nn'} = -t_{nn'} \begin{pmatrix} 0 & b_{nn'} \\ b_{n'n}^* & 0 \end{pmatrix} \]
\[ [S, [S, H^{ex}]]_{nn} = 2 \sum_{n''} I_{nn''} \begin{pmatrix} -|b_{nn''}|^2 & 0 \\ 0 & |b_{nn''}|^2 \end{pmatrix}, \] (35)
where \( I_{nn''} = |t_{nn''}|^2/(2J) \). Keeping terms up to the second order with respect to \( t \) (and only site-diagonal part of the second order terms) we obtain
\[ \tilde{H}_{nn'} = -J \sigma^z \delta_{nn'} + t_{nn'} \begin{pmatrix} a_{nn'} & 0 \\ 0 & a_{n'n} \end{pmatrix} + \sum_{n''} I_{nn''} (m_n \cdot m_{n''} - 1) \sigma^z \delta_{nn'}, \] (36)
In the second quantization the Hamiltonian obtained has the form (ignoring the constant term)
\[ \tilde{H} = \sum_{nn'} t_{nn'} \begin{pmatrix} \cos \frac{\theta_n}{2} & \cos \frac{\theta_n'}{2} \\ \sin \frac{\theta_n}{2} e^{i(\phi_n' - \phi_n)} & -\sin \frac{\theta_n}{2} \end{pmatrix} d_n^\dagger d_{n'} + \sum_{nn'} I_{nn'} (m_n \cdot m_{n'}) d_n^\dagger d_{n'}, \] (37)
where \( d^\dagger (d) \) is the operator of creation (annihilation) of a spinless electron. Thus strong exchange between the electrons and the core spins generates effective short-range antiferromagnetic exchange between the core spins.

In conclusion, we formulated the Dynamical Mean Field Approximation equations for the double-exchange model with classical spins for arbitrary electron dispersion law, concentration and relation between the exchange and the electron bandwidth. In the vicinity of the paramagnetic-ferromagnetic transition critical temperature \( T_c \), these equations were reduced to a MF equation, describing a single spin in an effective field, proportional to the macroscopic magnetization, and we obtained explicit formula for the \( T_c \). For the semi-circular electron density of states we explicitly calculated the transition temperature as a function of the exchange interaction and electron concentration.

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[1] C. Zener, Phys. Rev. 82, 403 (1951).
[2] P. W. Anderson and H. Hasegawa, Phys. Rev. 100, 675 (1955).
[3] P. G. de Gennes, Phys. Rev. 118, 141 (1960).
[4] J. M. D. Coey, M. Viret, S. von Molnar, Adv. Phys. 48, 167 (1999).
[5] Yu. A. Izyumov and Yu. N. Skryabin, Physics-Uspekhi, 44, 109 (2001).
[6] M. Ziese, Rep. Prog. Phys. 65, 143 (2002).
[7] D. M. Edwards, Adv. Phys. 51, 1259 (2002).
[8] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
[9] N. Furukawa, cond-mat/9812066.
[10] N. Furukawa: in Physics of Manganites, ed. T. Kaplan and S. Mahanti (Plenum Publishing, New York, 1999).
[11] A. Chattopadhyay and A. J. Millis Phys. Rev. B 64, 024424 (2001); A. Chattopadhyay, S. Das Sarma, and A. J. Millis Phys. Rev. Lett. 87, 227202 (2001).
[12] J. M. Ziman, Models of Disorder (Cambridge University Press, Cambridge, 1979).
[13] A. C. Hewson, The Kondo Problem to Heavy Fermions, (Cambridge University Press, Cambridge, England, 1993).
[14] S. Doniach and E. H. Sondheimer, Green’s functions for solid state physicists (Imperial College Press, London, 1998).
[15] M. Auslender and E. Kogan, Phys. Rev. B 65, 012408 (2002); Physica A 302, 345 (2001).
[16] M. Auslender and E. Kogan, EuroPhys. Lett. 59, 277 (2002).
[17] J. H. Van Vleck, Rev. Mod. Phys. 34, 681 (1962).
[18] A. Chattopadhyay, A. J. Millis, and S. Das Sarma Phys. Rev. B 64, 012416 (2001).
[19] Yu. A. Izyumov, Physics-Uspekhi, 40, 445 (1997).