

Electronic susceptibility and Curie temperature of the double-exchange model within dynamical mean-field theory

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Due to its applications to the manganites, the double-exchange (DE) model has been intensively studied over the past ten years. An especially promising approach to investigate the DE model is dynamical mean-field theory (DMFT), which becomes exact in infinite dimension but accurately describes local quantum fluctuations in three dimensions. In this article, we use DMFT to solve the Bethe–Salpeter equation for the electronic susceptibility above T_C . Assuming a semicircular density-of-states, we obtain an analytic relation for T_C in the limit of large Hund’s coupling from the condition that the inverse electronic susceptibility vanishes. Our expression for T_C agrees with an earlier result based on the local-moment susceptibility and corrects a mistake in a result based on the self-consistent equation for the magnetization below T_C . © 2003 American Institute of Physics. [DOI: 10.1063/1.1556201]

With the rediscovery of the manganites almost 10 years ago,¹ the double-exchange (DE) model has been the subject of many theoretical studies. At least qualitatively, the DE model describes the electron-mediated interactions between Mn moments in ferromagnetic manganites. For example, the DE model accurately predicts the colossal drop of the resistivity below the Curie temperature T_C . One of the most promising avenues to study itinerant systems is dynamical mean-field theory (DMFT), which becomes exact in the limit of infinite dimension but accurately describes local quantum fluctuations in three dimensions.² However, most applications of DMFT to the DE model have been restricted to the ferromagnetic phase below T_C .^{3–5} Although recent DMFT studies have provided analytic results for the spin conductivity⁶ and spin-diffusion coefficient⁷ above T_C , no theory exists for the full magnetic susceptibility χ of the DE model. In this article, we evaluate the electronic portion of χ to obtain an analytic expression for T_C from the condition that $1/\chi^{\text{el}} \rightarrow 0$.

The Hamiltonian of the DE model can be written as

$$H = -t \sum_{\langle i,j \rangle} (c_{i\alpha}^\dagger c_{j\alpha} + c_{j\alpha}^\dagger c_{i\alpha}) - 2J_H \sum_i s_i \cdot \mathbf{S}_i, \quad (1)$$

where $c_{i\alpha}^\dagger$ and $c_{i\alpha}$ are the creation and destruction operators for an electron with spin α at site i , $s_i = (1/2)c_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta}$ is the electronic spin, \mathbf{S}_i is the spin of the local moment, and J_H is the Hund’s coupling between the local and electronic spins. As is customary, the local moments are treated classically. We shall study the DE model in the limit of large $J_H S$ for the semicircular density-of-states $\rho_0(\epsilon) = (8/$

$\pi W^2) \sqrt{W^2/4 - \epsilon^2}$, where $W = 4t\sqrt{z}$ is the full bandwidth. For large coordination number z , the hopping energy t scales as $1/\sqrt{z}$.

In imaginary time, the full susceptibility of the DE model is given by

$$\chi(\mathbf{q}, i\omega_m)_{\alpha\beta} = \int_0^\beta d\tau e^{i\omega_m\tau} \sum_i e^{-i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_1)} \times \langle T_\tau S_{\text{tot},i}^\alpha(\tau) S_{\text{tot},1}^\beta(0) \rangle, \quad (2)$$

where $\omega_m = 2m\pi T$, T_τ is the time-ordering operator, and $\mathbf{S}_{\text{tot},i} = \mathbf{S}_i + \mathbf{s}_i$ is the total spin at site i . Notice that $\chi(\mathbf{q}, i\omega_m)_{\alpha\beta} = \chi(\mathbf{q}, i\omega_m) \delta_{\alpha\beta}$ contains three sets of terms: the local-moment susceptibility, the electronic susceptibility, and the cross terms.

Our goal is to evaluate the static electronic susceptibility $\chi^{\text{el}} = \lim_{q \rightarrow 0, \omega \rightarrow 0} \chi^{\text{el}}(\mathbf{q}, i\omega_m = \omega + i\epsilon)$, where

$$\chi^{\text{el}}(\mathbf{q}, i\omega_m) = \frac{1}{4} \int_0^\beta d\tau e^{i\omega_m\tau} \sum_i e^{-i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_1)} \times \langle T_\tau c_{i\alpha}^\dagger(\tau) c_{i\beta}(\tau) c_{1\kappa}^\dagger c_{1\delta} \rangle \boldsymbol{\sigma}_{\alpha\beta}^z \boldsymbol{\sigma}_{\kappa\delta}^z. \quad (3)$$

As shown in Fig. 1(a), we may write $\chi^{\text{el}}(\mathbf{q}, i\omega_m) = \sum_{l,n} \chi_{ln}(\mathbf{q}, i\omega_m)$, where $\nu_{l,n} = (2n_{l,n} + 1)\pi T$ are Fermi–Matsubara frequencies. For a fixed ω_m , the matrix (in Matsubara space) $\underline{\chi}(\mathbf{q}, i\omega_m)$ obeys the Bethe–Salpeter equation

$$\underline{\chi}(\mathbf{q}, i\omega_m) = \underline{\chi}^{(0)}(\mathbf{q}, i\omega_m) + \underline{\chi}^{(0)}(\mathbf{q}, i\omega_m) \underline{\Gamma}(i\omega_m) \underline{\chi}(\mathbf{q}, i\omega_m), \quad (4)$$

where $\underline{\Gamma}(i\omega_m)$ is the vertex function and $\underline{\chi}^{(0)}(\mathbf{q}, i\omega_m)$ is the bare susceptibility.⁸ This relation is sketched in Fig. 1(b), where summations are performed over the internal Fermi frequencies ν_o and ν_p .

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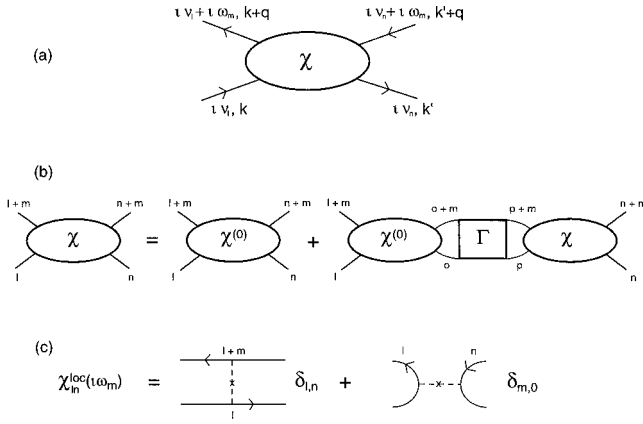


FIG. 1. Diagrams representing (a) the full susceptibility, (b) the Bethe–Salpeter equation, and (c) the local susceptibility with dashed lines connecting the center of each Green’s function to the local moment that is averaged over.

Within DMFT, momentum conservation at the internal vertices of irreducible graphs is disregarded so that internal Green’s functions are replaced by their local values. Consequently, the vertex function in Eq. (4) and Fig. 1(b) is independent of momenta and may be evaluated from an identical Bethe–Salpeter equation where $\chi(\mathbf{q}, i\omega_m)$ and $\chi^{(0)}(\mathbf{q}, i\omega_m)$ are replaced by *local* susceptibilities at site 1, obtained from the \mathbf{q} -dependent susceptibilities by summing over all \mathbf{q} . In other words, $\Gamma(i\omega_m) = \chi^{(0)-1}(\mathbf{q}, i\omega_m) - \chi^{-1}(\mathbf{q}, i\omega_m) = \chi^{loc(0)-1}(i\omega_m) - \chi^{loc-1}(i\omega_m)$.⁸

Defining $G_{\alpha\beta}^{loc}(i\nu_l)$ as the local Green’s function for a fixed orientation $\hat{\mathbf{m}}$ of the local moment, we obtain the local susceptibilities

$$\chi_{ln}^{loc(0)}(i\omega_m) = -\frac{T}{4} \delta_{ln} \langle G_{\delta\alpha}^{loc}(i\nu_l) \rangle \times \langle G_{\beta\kappa}^{loc}(i\nu_l + i\omega_m) \rangle \sigma_{\alpha\beta}^z \sigma_{\kappa\delta}^z, \quad (5)$$

$$\chi_{ln}^{loc}(i\omega_m) = -\frac{T}{4} \{ \delta_{ln} \langle G_{\delta\alpha}^{loc}(i\nu_l) G_{\beta\kappa}^{loc}(i\nu_l + i\omega_m) \rangle - \delta_{m,0} \langle G_{\beta\alpha}^{loc}(i\nu_l) G_{\delta\kappa}^{loc}(i\nu_n) \rangle \} \sigma_{\alpha\beta}^z \sigma_{\kappa\delta}^z, \quad (6)$$

where expectation values denote averages over $\hat{\mathbf{m}}$. Equation (6) is represented graphically by Fig. 1(c), where “ x ” denotes the local moment and a dashed line indicates that two Green’s functions are correlated by an average over $\hat{\mathbf{m}}$. In terms of the \mathbf{q} -dependent Green’s function $G_{\alpha\beta}(\mathbf{q}, i\nu_l)$, the bare \mathbf{q} -dependent susceptibility required in Eq. (4) is

$$\chi_{ln}^{(0)}(\mathbf{q}, i\omega_m) = -\frac{T}{4N} \delta_{ln} \sum_{\mathbf{k}} \langle G_{\delta\alpha}(\mathbf{k}, i\nu_l) \rangle \times \langle G_{\beta\kappa}(\mathbf{k} + \mathbf{q}, i\nu_l + i\omega_m) \rangle \sigma_{\alpha\beta}^z \sigma_{\kappa\delta}^z. \quad (7)$$

In the bare susceptibilities of Eqs. (5) and (7), the averages over $\hat{\mathbf{m}}$ are performed separately for each Green’s function.

The local and \mathbf{q} -dependent Green’s functions were first derived by Furukawa.⁴

$$G_{\alpha\beta}^{loc}(i\nu_l) = \frac{G_0^{-1}(i\nu_l) \delta_{\alpha\beta} - J_H S \sigma_{\alpha\beta} \cdot \hat{\mathbf{m}}}{G_0^{-2}(i\nu_l) - (J_H S)^2}, \quad (8)$$

$$\langle G_{\alpha\beta}(\mathbf{q}, i\nu_l) \rangle = \delta_{\alpha\beta} [i\nu_l + \mu - \epsilon_{\mathbf{q}} - (J_H S)^2 G_0(i\nu_l)]^{-1}, \quad (9)$$

where $G_0(i\nu_l) = 1/[i\nu_l + \mu - W^2 \langle G_{zz}^{loc}(i\nu_l) \rangle / 16]$ plays the role of a “mean field.”²

When $J_H S$ is much larger than both W and T , it is straightforward to show that the susceptibilities with $\omega_m = 0$ become $\chi_{ln}^{loc(0)} = -\delta_{ln} T / 2f_n^2$, $\chi_{ln}^{loc} = (1 - \delta_{ln}) T / 3f_l f_n$, and

$$\chi_{ln}^{(0)}(\mathbf{q}=0) = \frac{4T}{W^2} \delta_{ln} \left\{ 1 - \frac{8}{W^2} f_n \left(z_n + \frac{1}{2} f_n \right) \right\}^{-1}, \quad (10)$$

where $f_n = z_n + \sqrt{z_n^2 - W^2/8}$ and $z_n = i\nu_n + \delta\mu$. Here, $\delta\mu = \mu \pm J_H S$ for band filling p less than (+) or greater than (–) 1, corresponding to one electron per site or a completely filled lower band.

Of course, both $\chi^{loc(0)}$ and $\chi^{(0)}(\mathbf{q}=0)$ can be immediately inverted because each is proportional to the unit matrix. If χ^{loc} is a $2n_\chi \times 2n_\chi$ matrix with $|\nu_{l,n}| \leq (2n_\chi - 1)\pi T$, then its inverse is given by

$$\chi_{ln}^{loc-1} = \frac{3}{T} \left\{ -\delta_{ln} f_l^2 + \frac{f_l f_n}{2n_\chi - 1} \right\}. \quad (11)$$

It follows that the inverse of the full electronic susceptibility matrix with $\omega_m = 0$ is

$$\chi_{ln}^{-1}(\mathbf{q}=0) = \frac{1}{T} \left[\delta_{ln} \left(\frac{W^2}{4} - 2f_l(z_l + f_l) \right) + \frac{3}{2n_\chi - 1} f_l f_n \right]. \quad (12)$$

The condition for T_C that $\chi^{el} = \sum_{l,n} \chi_{ln}(\mathbf{q}=0) \rightarrow \infty$ implies that $\det[\chi^{-1}(\mathbf{q}=0)] \rightarrow 0$. With $R_n = (\sqrt{z_n^2 - W^2/8} - z_n)/2$, T_C is implicitly given by the relation

$$\sum_n \frac{R_n^2}{R_n^2 - 3W^2/32} = 1. \quad (13)$$

Also in the limit of large $J_H S$, the band filling is given by

$$p = 1 + \frac{1}{2} \text{sgn}(p-1) + 2T \sum_n \text{Re} \left\{ \frac{1}{f_n} \right\}. \quad (14)$$

These results agree with Furukawa⁴ except for a corrected definition of R_n .⁹ Notice that Eq. (13) is independent of the size of χ^{loc} .

In the limit $T_C \ll W$, replacing the Matsubara sums in Eqs. (13) and (14) by integrals yields the analytic expressions

$$T_C = \frac{W\sqrt{2}}{8\pi} \left\{ \sqrt{1-y^2} - \frac{1}{\sqrt{3}} \tan^{-1} \sqrt{3(1-y^2)} \right\}, \quad (15)$$

$$p = 1 + \frac{1}{2} \text{sgn}(p-1) + \frac{1}{\pi} \{ y \sqrt{1-y^2} + \sin^{-1} y \}, \quad (16)$$

where $y = 2\sqrt{2} \delta\mu / W$. These results are identical to those of Auslender and Kogan,¹⁰ who evaluated the local-moment susceptibility by integrating over the Fermionic degrees of freedom.

Results for T_C/W from Eqs. (13) and (15) are plotted in Fig. 2 for $0 \leq p \leq 1$. Symmetric results are obtained for $1 \leq p \leq 2$. Since the maximum T_C at half filling ($p = 1/2$) is

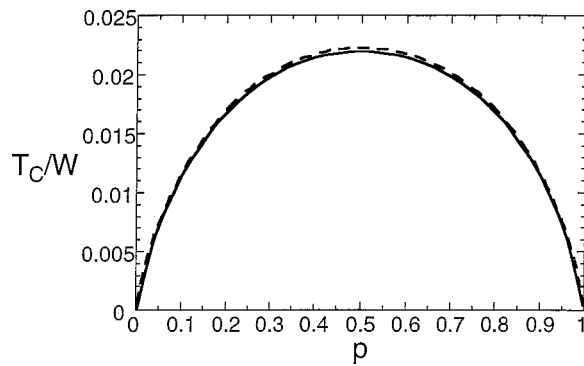


FIG. 2. Results for T_C/W from Eqs. (13) (solid) and (15) (dashed) vs band-filling p .

about $0.022 W$, the approximation $T_C \ll W$ is certainly justified. Hence, we have established that the Curie temperature can be evaluated consistently from the divergence of either the local moment or electronic portions of the magnetic susceptibility above T_C as well as from a self-consistent relation for the magnetization below T_C .

In future work, we shall generalize the present approach to include all sets of terms in the full susceptibility of Eq. (2). However, our calculation, like all previous ones, ignores

the quantum corrections due to the local mutual precession of the electronic and local magnetic moments. These quantum corrections persist even in the $z \rightarrow \infty$ limit when S is finite.

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