Thermodynamic consistency of the dynamical mean-field theory of the double-exchange model

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We find that standard diagrammatic perturbation theory does not exist for the dynamical mean-field theory of the double-exchange model because the vertex function cannot be expanded in terms of the bare vertex function and the full Green’s function $G(i\nu_n)_{\alpha\alpha}$. Nevertheless, a functional $\Pi$ satisfying the condition $\delta \Pi / \delta G(i\nu_n)_{\alpha\alpha} = \Sigma(i\nu_n)_{\alpha\alpha}$ can be constructed because the curl of the self-energy with respect to the Green’s function vanishes: $\delta \Sigma(i\nu_n)_{\alpha\alpha} / \delta (i\nu)_{\beta\beta} = \delta (i\nu)_{\beta\beta} / \delta G(i\nu_n)_{\alpha\alpha} = 0$. The connection between the functional $\Pi$ and the free energy implies that the theory is thermodynamically consistent, meaning that the same thermodynamic properties may be obtained from either the partition function or the Green’s function. We provide a concrete example of this consistency by evaluating the magnetic susceptibility and Curie temperature for any Hund’s coupling using two such approaches.

The dynamical mean-field theory (DMFT) formulated in the late 1980s by Müller-Hartmann,1 and Metzner and Vollhardt2 has developed into one of the most powerful many-body techniques for studying electronic models such as the Hubbard3,4 and double-exchange5–9 (DE) models. This theory is believed to become exact in the limit of infinite dimensions and to capture the physics of correlated electron systems even in three dimensions. Recent work on dilute magnetic semiconductors has used DMFT to study variants of the DE model10,11 with less than one local moment per site. In this paper, we reach the surprising conclusion that, unlike for the DMFT of the Hubbard model,2 a diagrammatic perturbation theory containing only electronic degrees of freedom does not exist for the DMFT of the DE model. Nevertheless, we show that the theory remains $\Pi$ derivable in a more restrictive sense, which still implies that the partition function and Green’s function produce consistent results for thermodynamic properties such as the magnetic susceptibility and Curie temperature. This provides an example of an electronic theory that is thermodynamically consistent despite the absence of a weak-coupling, diagrammatic perturbation theory.

The Hamiltonian of the DE model is given by

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger \sigma_{\alpha\beta} c_j + c_j^\dagger \sigma_{\beta\alpha} c_i) - 2J_H \sum_i s_i \cdot S_i,$$

(1)

where $c_{i\alpha}$ and $c_{i\beta}$ are the creation and destruction operators for an electron with spin $\alpha$ at site $i$, $s_{i\alpha} = (1/2) c_i^\dagger \sigma_{\alpha\beta} c_i$ is the electronic spin, and $S_i = \sum_m s_m$ is the spin of the local moment, which is going to be treated as a classical field. Repeated spin indices are summed. The DE model is believed to provide a qualitative description of magnetoresistive materials,12 where the electronic conductivity is promoted by the alignment of the local spins below $T_C$. Within DMFT, the local effective action above $T_C$ in zero field is given by

$$A_{eff}(\mathbf{m}) = -T \sum_n \bar{c}_{0n}(i\nu_n)[G_0(i\nu_n)^{-1} \delta_{\alpha\beta} + J_H \sigma_{\alpha\beta} \cdot \mathbf{m}]c_{0n}(i\nu_n),$$

(2)

where $\bar{J}_H = J_H S$, $\nu_n = (2n+1)\pi T$, $\bar{c}_{0n}(i\nu_n)$ and $c_{0n}(i\nu_n)$ are now anticommuting Grassman variables, and $G_0(i\nu_n)$ is the bare Green’s function containing dynamical information about the hopping of electrons from other sites onto the site 0. Because $A_{eff}(\mathbf{m})$ is quadratic in the Grassman variables, the full local Green’s function $G(i\nu_n)_{\alpha\beta}$ may be readily solved by integrating over the Grassman variables, with the paramagnetic result

$$G(i\nu_n) = G(i\nu_n)_{\alpha\alpha} = \langle \{ G_0(i\nu_n)^{-1} + \bar{J}_H \sigma \cdot \mathbf{m} \}^{-1} \rangle_m = \frac{G_0(i\nu_n)^{-1}}{G_0(i\nu_n)^{-2} - \bar{J}_H^2},$$

(3)

where $I$ is the unity matrix in $2 \times 2$ spin space. The average over the orientations $\mathbf{m}$ of the local moment is generally given by $\langle C(\mathbf{m}) \rangle_m = \int d\Omega_m P(\mathbf{m}) C(\mathbf{m})$, where $P(\mathbf{m}) \propto \text{Tr}(\exp(-A_{eff}(\mathbf{m})))$ is the probability for the local moment to point in the $\mathbf{m}$ direction. Above $T_C$, $P(\mathbf{m}) = 1/4\pi$ is constant. Consequently, the paramagnetic self-energy is given by

$$\Sigma(i\nu_n) = G_0(i\nu_n)^{-1} - G(i\nu_n)^{-1} = \bar{J}_H G_0(i\nu_n).$$

Expanding in powers of $\bar{J}_H$ and $G(i\nu_n)$, we find

$$\Sigma(i\nu_n) = \frac{1}{2G(i\nu_n)} + \sqrt{\frac{1}{4G(i\nu_n)^2} + \bar{J}_H^2}$$

$$= \bar{J}_H G(i\nu_n) - \bar{J}_H^2 G(i\nu_n)^3 + 2\bar{J}_H^3 G(i\nu_n)^5 + \cdots$$

(4)

On a Bethe lattice, these relations are closed by the analytic expression$^4,5$
where $z_n = iv_n + \mu$ and $W$ is the full bandwidth of the noninteracting, semicircular density of states. We denote the full spin dependence for later use.

Diagrammatic perturbation theory is customarily formulated in terms of the bare vertex function $\Gamma^{(0)}(l, l; m)^{\alpha\beta;0}$. sketched in Fig. 1(a) with $\omega_n = 2m\pi T$. The bare vertex function may be associated with the two-particle interaction in the purely electronic effective action

$$\begin{align*}
A^e_{\text{eff}} &= - T \sum_n \bar{c}_{0a}(iv_n) G_0(iv_n)^{-1} c_{0a}(iv_n) - \frac{T^2}{4} \sum_{l, n, m} \bar{c}_{0a}(iv_n) \\
&\quad + i \omega_n c_{0b}(iv_n) \Gamma^{(0)}(l, n; m)^{\alpha\beta;0} c_{0b}(iv_n) c_{0a}(iv_n + i \omega_n) .
\end{align*}$$

(6)

Hence, the bare vertex function must satisfy the crossing symmetries $\Gamma^{(0)}(l, l + m; n - l)^{\alpha\beta;0} = \Gamma^{(0)}(n + m, n; l - n)^{\alpha\beta;0} = - \Gamma^{(0)}(l, n; m)^{\alpha\beta;0}$. There are two ways to calculate $\Gamma^{(0)}(l, n; m)^{\alpha\beta;0}$. First, we can take the limit of the full irreducible vertex $\Gamma(l, n; m)^{\alpha\beta;0}$ obtained from the Bethe-Salpeter equation for the magnetic susceptibility. Alternatively, we can associate the lowest-order, $J_H$ contribution to the partition function $Z = \langle \text{Tr} \exp(-A^e_{\text{eff}}(\mathbf{m})) \rangle / \text{m}$ with the contribution to the partition function $Z' = \langle \text{Tr} \exp(-A^e_{\text{eff}}(\mathbf{m})) \rangle$, sketched as the compact diagram in Fig. 1(b) with the formal lines given by the bare Green’s functions $G_0(iv_n)^{\alpha\beta}$. Both methods yield the same result,

$$\begin{align*}
\Gamma^{(0)}(l, n; m)^{\alpha\beta;0} &= \frac{1}{3} \sum_{l, n} \bar{c}_{0n} \Gamma^{(0)}(l, n; m)^{\alpha\beta;0} c_{0n} - \bar{c}_{0n} \Gamma^{(0)}(l, n; m)^{\alpha\beta;0} c_{0n} .
\end{align*}$$

(7)

which satisfies the crossing symmetries.

However, replacing $A^e_{\text{eff}}(\mathbf{m})$ by $A^e_{\text{eff}}$ produces an inequivalent theory. For example, expanding $Z$ and $Z'$ in powers of $J_H$ yields the results

$$\begin{align*}
Z &= Z_0 \left\{ 1 - \frac{T^2}{2} \sum_n G_0(iv_n)^2 + \frac{T^2}{2} \sum_{l, n} \bar{c}_{0n} G_0(iv_n)^2 c_{0n} + \mathcal{O}(J_H^4) \right\} ,
\end{align*}$$

(8)

$$\begin{align*}
Z' &= Z_0 \left\{ 1 - \frac{T^2}{2} \sum_n G_0(iv_n)^2 + \frac{T^2}{6} \sum_{l, n} \bar{c}_{0n} G_0(iv_n)^2 c_{0n} + \mathcal{O}(J_H^4) \right\} ,
\end{align*}$$

(9)

which disagree to order $J_H$. Hence, it is not possible by averaging over the local moments to replace the Hund’s coupling with an effective two-particle interaction between the electrons. In other words, the Hund’s coupling produces fourth and higher-derder interaction that require higher-order vertex functions in the electronic action.

A theory is usually said to be $\Phi$ derivable if a functional $\Phi \{ G(iv_n) \} $, constructed from the sum of compact diagrams in terms of the full Green’s functions and the bare vertex functions, can be found to satisfy the condition $\Sigma (iv_n)^{\alpha\beta} = \delta \Phi / \delta G(iv_n)^{\alpha\beta}$. As discussed by Baym, a $\Phi$-derivable theory may readily be shown to be thermodynamically consistent, meaning that thermodynamic properties can be evaluated either from the Green’s function or from the partition function. Consequently, such a theory is consistent on the one- and two-particle levels. We emphasize that it is the theory of a model that may be thermodynamically consistent, not the model Hamiltonian itself. For a $\Phi$-derivable theory, the partition function $Z$ or free energy $-T \ln Z$ may be constructed in terms of $\Phi$ from the relation

$$\begin{align*}
- T \ln Z &= \sum_n \text{Tr} \{ \Sigma (iv_n) G_0(iv_n) \} + \sum_n \text{Tr} \ln \{ G_0(iv_n) \} ,
\end{align*}$$

(10)

which is stationary under variations of $G(iv_n)$. Whereas Baym’s original work was intended for systems of interacting fermions and bosons, the notion of $\Phi$ derivability has been extended to systems of interacting electrons and spins and to disordered alloys.
Eq. (3) and Dyson’s equation for the self-energy, we find that
\[ \frac{\partial \Sigma(i\nu_n)_{a\alpha}}{\partial G(i\nu_n)_{b\beta}} = (K^{-1})^{a\alpha \beta}_{in} + \delta_{a\alpha} \delta_{a\alpha} G(i\nu_n)^{-2}, \]
where \( K \) is the Jacobian
\[ e^{\alpha}_{in} = \frac{\partial G(i\nu_n)_{b\beta}}{\partial G(i\nu_n)_{a\alpha}} \]
\[ = \delta_{a\alpha} \left\{ \frac{2 \tilde{J}_H}{3} b_n \delta_{a\beta} \right\} + \frac{\tilde{J}_H}{3} \delta_{a\beta} (2 \delta_{a\beta} - 1), \]
with \( a_n = G(i\nu_n)^{-2} \tilde{J}_H \) and \( b_n = G(i\nu_n)^{-2} - \tilde{J}_H^2 / 3 \). This Jacobian can be inverted with the general result
\[ \frac{\partial \Sigma(i\nu_n)_{a\alpha}}{\partial G(i\nu_n)_{b\beta}} = \delta_{a\alpha} \left\{ \frac{2}{2a_n - 3b_n} + \delta_{a\alpha} G(i\nu_n)^2 \right\} - \frac{\tilde{J}_H}{3} \frac{a_d a\alpha}{2} (2 \delta_{a\beta} - 1). \]

It can be shown that the right-hand side equals \(-T^T(l,n,m=0)_{a\alpha \beta} \) where \( \Gamma(l,n,m)_{a\alpha \beta} \) is the full irreducible vertex of the Bethe-Salpeter equation. The functional \( \Phi \) must exist because the curl of the self-energy vanishes:
\[ \frac{\partial \Sigma(i\nu_n)_{a\alpha}}{\partial G(i\nu_n)_{b\beta}} - \frac{\partial \Sigma(i\nu_n)_{b\beta}}{\partial G(i\nu_n)_{a\alpha}} = 0. \]

By construction, \( \Phi^{(1)} \) (second order in \( \tilde{J}_H \)) is represented by the compact diagram in Fig. 1(b) and is given in terms of the bare vertex function by
\[ \Phi^{(1)} = -\frac{T}{2} \sum_{l,r} \Gamma^{(0)}(l,r;0)_{a\alpha \beta} G(i\nu_n)_{a\alpha} G(i\nu_r)_{b\beta} = -\frac{\tilde{J}_H}{6} \sum_{n} \left\{ \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)_{a\alpha} G(i\nu_n)_{a\alpha} - G(i\nu_n)_{a\alpha} \right\} - \frac{\tilde{J}_H}{6} \sum_{n} \left\{ \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)_{a\alpha} G(i\nu_n)_{a\alpha} - G(i\nu_n)_{a\alpha} \right\} - \frac{\tilde{J}_H}{6} \sum_{n} \left\{ \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)_{a\alpha} G(i\nu_n)_{a\alpha} - G(i\nu_n)_{a\alpha} \right\} \right\} \]
where \( \bar{a} \) is the opposite spin to \( a \). After expanding and integrating Eq. (12),\(^{19} \) we find that \( \Phi^{(2)} \) (fourth order in \( \tilde{J}_H \)) is given by
\[ \Phi^{(2)} = \frac{\tilde{J}_H}{9} \left\{ \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)^2_{a\alpha} - \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)^2_{a\alpha} - \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)^2_{a\alpha} \right\} \]
\[ + \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)^2_{a\alpha} - \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)^2_{a\alpha} \right\} \]
\[ + \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)^2_{a\alpha} - \frac{1}{2} \sum_{a\alpha \beta} G(i\nu_n)^2_{a\alpha} \right\} \]
Unlike \( \Phi^{(1)}, \Phi^{(2)} \) cannot be represented by a compact diagram involving only the bare vertex functions. So far, all of our results are valid for any lattice topology (including the Bethe and hypercubic lattices in infinite dimensions).

We have verified the thermodynamic consistency of the DMFT by calculating the magnetic susceptibility from both the Green’s function and the partition function. With a magnetic field \( H = Hz \) coupled to both the local moments and the electrons, the effective action becomes
\[ A_{\text{eff}}(m) = -T \sum_n \bar{c}_{0\alpha}(i\nu_n) \left\{ \left( G_0(i\nu_n)_{a\alpha} - 2 \tilde{J}_H \sigma_{a\alpha} \right) \right\} \times c_{0\beta}(i\nu_n) - \beta H S_{\text{m}}. \]
In a field, \( G_0(i\nu_n) \) is no longer proportional to the identity matrix in spin space but on a Bethe lattice is still related to \( G(i\nu_n) \) by Eq. (5).

Parametrizing the bare inverse Green’s function as
\[ G_0(i\nu_n)_{a\alpha} = (\epsilon_n + R_n)I + Q_n \sigma_{a\alpha}, \]
and using Eq. (5), we solve for \( R_n \) and \( Q_n \) from the expression
\[ R_n + Q_n \sigma_{a\alpha} = - \frac{W^2}{16} ((\epsilon_n + R_n)I + Q_n \sigma_{a\alpha}). \]
To linear order in the field, \( R_n \) and \( Q_n \) satisfy the implicit relations
\[ R_n = \frac{W^2}{16} \frac{\epsilon_n + R_n}{(\epsilon_n + R_n)^2 - \tilde{J}_H^2}, \]
\[ Q_n = \frac{H}{2} \frac{(\epsilon_n + R_n)^2 - \tilde{J}_H^2}{(\epsilon_n + R_n)^2 - \tilde{J}_H^2}. \]
where
\[ U_n = 1 - \frac{32 \tilde{J}_H}{3W^2} \frac{R_n^2}{(\epsilon_n + R_n)(\epsilon_n + R_n + 2R_n)}. \]

After integrating \( \exp(-A_{\text{eff}}(m)) \) over the Grassman variables, we find that the probability for the local moment to point along \( m \) is
\[ P(m) \propto \exp \left\{ \frac{1}{2} \sum_n \ln \left( 1 - \frac{\tilde{J}_H}{2} \sigma_{a\alpha} \right) \right\} - \beta \Sigma_{\text{eff}}(m) \]
\[ \propto \exp(\beta \Sigma_{\text{eff}}(m) \sigma_{a\alpha}). \]
The last relation is written to lowest order in the local-moment order parameter \( M_{\text{m}} = \langle m \rangle_{\bar{m}} \) and defines the effective interaction
\[ J_{\text{eff}} = \frac{16T \tilde{J}_H}{W^2} \sum \frac{R_n}{(\epsilon_n + R_n)(\epsilon_n + R_n + 2R_n)} \left\{ \langle x \rangle_{\text{m}}(\epsilon_n + R_n)^2 - \tilde{J}_H R_n \right\} \]
\[ + \chi^{-1} S, \]
where \( \chi_{\text{m}} = M_{\text{m}} / H \) is the local-moment susceptibility. Now \( M_{\text{m}} \) is solved from the condition \( M_{\text{m}} = J_{\text{eff}} M_{\text{m}} \beta / 3 \), which contains terms proportional to both \( H \) and \( M_{\text{m}} \) on the right-hand side. The electronic order parameter \( M_a = 2(\bar{q})_{ab} \) is obtained from the summation \( M_a = -(32T / W^2) \sum_a Q_a \). The total-spin susceptibility is then given by the zero-field limit of \( \chi = (S M_{\text{m}} + M_e / 2) / H \).

To calculate the susceptibility from the partition function, we first expand \( Z \) to the second order in \( H \) and \( M_{\text{m}} \) and then use \( \chi = (T / H) F \ln Z / \partial H |_{\bar{m}=0} \). The latter technique is formally equivalent to evaluating the susceptibility from the Bethe-Salpeter equation.\(^8 \)
These two sets of calculations do indeed produce the same magnetic susceptibility, which may be written as

$$\chi = \frac{S_{\text{eff}}(T)^2}{3T - (J_H/W)^2} + \frac{3T}{4W^2} (G_1(T) - G_2(T))$$

$$+ \frac{8J_H^2}{W^4} G_1(T),$$

(22)

$$S_{\text{eff}}(T) = S + \frac{3J_H^2}{2W^2} (G_1(T) - G_2(T)),$$

(23)

where the functions $G_1(T)$ and $G_2(T)$ are formally given by the Matsubara sums

$$G_1(T) = -\frac{32}{3} \sum_n \frac{R_n^2}{(\varepsilon_n + R_n)(\varepsilon_n + 2R_n)U_n},$$

(24)

$$G_2(T) = -\frac{32}{3} \sum_n \frac{R_n}{(\varepsilon_n + R_n)U_n}. $$

(25)

The Curie temperature $T_C$ is solved from the condition $G_1(T_C) = (W/|J_H|)^2$. The identical results produced by these two calculations of the magnetic susceptibility and Curie temperature provide a concrete example of the thermodynamic consistency of the DMFT of the DE model. Thus, any thermodynamic quantity can be evaluated either from the Green’s function (on the one-particle level) or the partition function (containing interactions on the two-particle level). Diagrammatics may be recovered for a more sophisticated model where the classical local moments are replaced by fully quantum-mechanical operators and we introduce an additional propagator corresponding to those local spins. It may also be possible to develop a more complex diagrammatics for classical local spins in terms of higher-order vertex functions.

Finally, we note that whereas any conserving theory (in the sense of Baym and Kadanoff\textsuperscript{19}) is thermodynamically consistent, it is not true that all thermodynamically consistent theories are conserving. Indeed, that is the case here since the DMFT violates the Ward identities associated with charge and spin conservation.

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4. Applications of DMFT to the Hubbard model and additional references are contained in the comprehensive review article: A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
15. The electronic effective action $A'_{\text{eff}}$ would still produce an inequivalent theory even if the three-dimensional local spins $\mathbf{S}_m$ were replaced by Ising spins $\pm \mathbf{S}_z$.
19. Due to the term containing $\{1 - (2/3)J_H^2\Sigma_{\mathbf{r}}(G_3(\mathbf{r}))\}^{-2} - J_H^2(3)^{-1}$ in the irreducible vertex function $\Gamma$, the radius of convergence in powers of $J_H$ is of order $T$. In the limit $J_H \rightarrow \infty$, $\Gamma$ depends on the cutoff $n_s$ of the Matsubara sum (Ref. 8).
20. In the $J_H \rightarrow \infty$ limit, $G_1(T) \rightarrow (W/|J_H|)^2 F_1(T)$ and $G_2(T) \rightarrow (W^2/3|J_H|)[|p-1|-1-2 \text{sgn}(p-1)F_2(T)]$, where $F_1(T)$ and $F_2(T)$ were defined in Ref 8.