

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

Randy S. Fishman,¹ Juana Moreno,² Thomas Maier,³ and Mark Jarrell⁴

¹Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6032, USA

²Physics Department, University of North Dakota, Grand Forks, North Dakota 58202-7129, USA

³Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6032, USA

⁴Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221, USA

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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 $G(i\nu)_{\alpha\alpha}$. Nevertheless, a functional Φ satisfying the condition $\delta\Phi/\delta G(i\nu)_{\alpha\alpha} = \Sigma(i\nu)_{\alpha\alpha}$ can be constructed because the curl of the self-energy with respect to the Green's function vanishes: $\delta\Sigma(i\nu)_{\alpha\alpha}/\delta G(i\nu)_{\beta\beta} - \delta\Sigma(i\nu)_{\beta\beta}/\delta G(i\nu)_{\alpha\alpha} = 0$. The connection between the functional Φ 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.

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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 Hubbard^{3,4} 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 model^{10,11} 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,⁴ 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 Φ 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

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

where $c_{i\alpha}^\dagger$ and $c_{i\alpha}$ are the creation and destruction operators for an electron with spin α at site i , $\mathbf{s}_i = (1/2)c_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta}$ is the electronic spin, and $\mathbf{S}_i = S\mathbf{m}_i$ 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

$$A_{\text{eff}}(\mathbf{m}) = -T \sum_n \bar{c}_{0\alpha}(i\nu_n) \{ G_0(i\nu_n)^{-1} \delta_{\alpha\beta} + \tilde{J}_H \boldsymbol{\sigma}_{\alpha\beta} \cdot \mathbf{m} \} c_{0\beta}(i\nu_n), \quad (2)$$

where $\tilde{J}_H = J_H S$, $\nu_n = (2n+1)\pi T$, $\bar{c}_{0\alpha}(i\nu_n)$ and $c_{0\alpha}(i\nu_n)$ 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 $A_{\text{eff}}(\mathbf{m})$ is quadratic in the Grassman variables, the full local Green's function $G(i\nu)_{\alpha\beta}$ may be readily solved by integrating over the Grassman variables, with the paramagnetic result⁵

$$\begin{aligned} \underline{G}(i\nu_n) &= G(i\nu_n) \underline{I} = \langle \{ G_0(i\nu_n)^{-1} \underline{I} + \tilde{J}_H \boldsymbol{\sigma} \cdot \mathbf{m} \}^{-1} \rangle_{\mathbf{m}} \\ &= \frac{G_0(i\nu_n)^{-1}}{G_0(i\nu_n)^{-2} - \tilde{J}_H^2} \underline{I}, \end{aligned} \quad (3)$$

where \underline{I} is the unity matrix in 2×2 spin space. The average over the orientations \mathbf{m} of the local moment is generally given by $\langle C(\mathbf{m}) \rangle_{\mathbf{m}} = \int d\Omega_{\mathbf{m}} P(\mathbf{m}) C(\mathbf{m})$, where $P(\mathbf{m}) \propto \text{Tr}(\exp(-A_{\text{eff}}(\mathbf{m})))$ 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 $\Sigma(i\nu_n) = G_0(i\nu_n)^{-1} - G(i\nu_n)^{-1} = \tilde{J}_H^2 G_0(i\nu_n)$. Expanded in powers of \tilde{J}_H and $G(i\nu_n)$, we find

$$\begin{aligned} \Sigma(i\nu_n) &= -\frac{1}{2G(i\nu_n)} + \sqrt{\frac{1}{4G(i\nu_n)^2} + \tilde{J}_H^2} \\ &= \tilde{J}_H^2 G(i\nu_n) - \tilde{J}_H^4 G(i\nu_n)^3 + 2\tilde{J}_H^6 G(i\nu_n)^5 + \dots \end{aligned} \quad (4)$$

On a Bethe lattice, these relations are closed by the analytic expression^{4,5}

$$G_0(i\nu_n)^{-1} = z_n I - \frac{W^2}{16} G(i\nu_n), \quad (5)$$

where $z_n = i\nu_n + \mu$ 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 $\Gamma^{(0)}(l, n; m)^{\beta\alpha; \delta\kappa}$ sketched in Fig. 1(a) with $\omega_m = 2m\pi T$. The bare vertex function may be associated with the two-particle interaction in the purely electronic effective action¹³

$$A'_{\text{eff}} = -T \sum_n \bar{c}_{0\alpha}(i\nu_n) G_0(i\nu_n)^{-1} c_{0\alpha}(i\nu_n) - \frac{T^3}{4} \sum_{l, n, m} \bar{c}_{0\alpha}(i\nu_n + i\omega_m) c_{0\beta}(i\nu_n) \Gamma^{(0)}(l, n; m)^{\beta\alpha; \delta\kappa} \bar{c}_{0\kappa}(i\nu_l) c_{0\delta}(i\nu_l + i\omega_m). \quad (6)$$

Hence, the bare vertex function must satisfy the crossing symmetries $\Gamma^{(0)}(l, l+m; n-l)^{\delta\alpha; \beta\kappa} = \Gamma^{(0)}(n+m, n; l-n)^{\beta\kappa; \delta\alpha} = -\Gamma^{(0)}(l, n; m)^{\beta\alpha; \delta\kappa}$. There are two ways to calculate $\Gamma^{(0)} \times (l, n; m)^{\beta\alpha; \delta\kappa}$. First, we can take the $J_H \rightarrow 0$ limit of the full irreducible vertex $\Gamma(l, n; m)^{\beta\alpha; \delta\kappa}$ obtained from the Bethe-Salpeter equation for the magnetic susceptibility.^{8,14} Alternatively, we can associate the lowest-order, J_H^2 contribution to the partition function $Z = \langle \text{Tr}(\exp(-A_{\text{eff}}(\mathbf{m}))) \rangle_{\mathbf{m}}$ with the contribution to the partition function $Z' = \text{Tr}(\exp(-A'_{\text{eff}}))$, sketched as the compact diagram in Fig. 1(b) [with internal lines given by the bare Green's functions $G_0(i\nu_n)_{\alpha\beta}$]. Both methods yield the same result,

$$\Gamma^{(0)}(l, n; m)^{\beta\alpha; \delta\kappa} = \frac{1}{3} \beta \tilde{J}_H^2 \{ \sigma_{\beta\alpha} \cdot \sigma_{\delta\kappa} \delta_{m,0} - \sigma_{\delta\alpha} \cdot \sigma_{\beta\kappa} \delta_{ln} \}, \quad (7)$$

which satisfies the crossing symmetries.

However, replacing $A_{\text{eff}}(\mathbf{m})$ by A'_{eff} produces an inequivalent theory.¹⁵ For example, expanding Z and Z' in powers of J_H yields the results

$$Z = Z_0 \left\{ 1 - \tilde{J}_H^2 \sum_n G_0(i\nu_n)^2 + \frac{1}{2} \tilde{J}_H^4 \sum_{l \neq n} G_0(i\nu_l)^2 G_0(i\nu_n)^2 + \mathcal{O}(\tilde{J}_H^6) \right\}, \quad (8)$$

$$Z' = Z_0 \left\{ 1 - \tilde{J}_H^2 \sum_n G_0(i\nu_n)^2 + \frac{5}{6} \tilde{J}_H^4 \sum_{l \neq n} G_0(i\nu_l)^2 G_0(i\nu_n)^2 + \mathcal{O}(\tilde{J}_H^6) \right\}, \quad (9)$$

which disagree to order \tilde{J}_H^4 . 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-order electronic interactions that require higher-order vertex functions in the electronic action.

A theory is usually said to be Φ derivable if a functional $\Phi(\{G(i\nu_n)\})$, constructed from the sum of compact diagrams in terms of the full Green's functions and the bare vertex

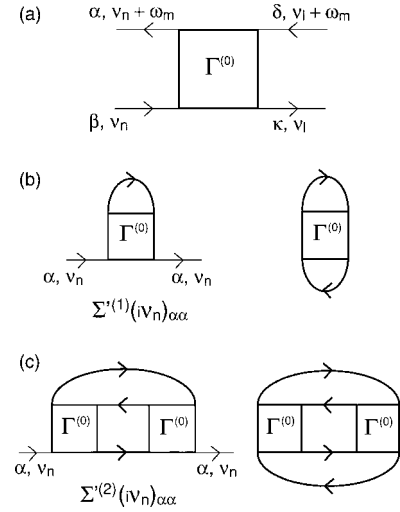


FIG. 1. (a) The bare vertex function; (b) and (c) compact diagrams that contribute to Φ for the electronic effective action A'_{eff} on the right with their associated self-energies on the left.

functions, can be found to satisfy the condition $\Sigma(i\nu_n)_{\alpha\beta} = \delta\Phi / \delta G(i\nu_n)_{\alpha\beta}$. As discussed by Baym,¹⁶ a Φ -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 Z . 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 Φ -derivable theory, the partition function Z or free energy $-T \ln Z$ may be constructed in terms of Φ from the relation

$$-\ln Z = \Phi - \sum_n \text{Tr}\{\Sigma(i\nu_n)G(i\nu_n)\} + \sum_n \text{Tr} \ln\{G(i\nu_n)\}, \quad (10)$$

which is stationary under variations of $G(i\nu_n)$. Whereas Baym's original work was intended for systems of interacting fermions and bosons, the notion of Φ derivability has been extended to systems of interacting electrons and spins¹⁷ and to disordered alloys.¹⁸

From the discussion above, it is clear that even if it exists, Φ cannot be constructed in terms of the bare vertex functions. When the action contains only two-particle interactions such as for the Hubbard model, then the first two terms in Φ are represented by the compact diagrams on the right-hand side of Figs. 1(b) and 1(c) with the corresponding self-energies $\Sigma(i\nu_n)_{\alpha\alpha} = \delta\Phi / \delta G(i\nu_n)_{\alpha\alpha}$ sketched on the left-hand side. Not surprisingly, substituting our earlier expression for the bare vertex function produces the correct first-order self-energy $\Sigma^{(1)}(i\nu_n) = \tilde{J}_H^2 G(i\nu_n)$ but the wrong second-order self-energy $\Sigma^{(2)}(i\nu_n) = -(\tilde{J}_H^4/3)\{2G(i\nu_n)\Sigma_l G(i\nu_l)^2 + G(i\nu_n)^3\}$. Notice from Eq. (4) that the correct second-order self-energy $\Sigma^{(2)}(i\nu_n) = -\tilde{J}_H^4 G(i\nu_n)^3$ does not involve a Matsubara summation. Hence, the DMFT of the DE model is not Φ derivable in the strict diagrammatic sense stated above.

Despite the failure of a diagrammatic expansion in powers of $\Gamma^{(0)}$, a functional $\Phi(\{G(i\nu_n)\})$ can still be constructed to satisfy the condition $\Sigma(i\nu_n)_{\alpha\alpha} = \delta\Phi / \delta G(i\nu_n)_{\alpha\alpha}$. Starting from

Eq. (3) and Dyson's equation for the self-energy, we find that $\delta\Sigma(i\nu_l)_{\alpha\alpha}/\delta G(i\nu_n)_{\beta\beta}=(\underline{K}^{-1})_{ln}^{\alpha\beta}+\delta_{ln}\delta_{\alpha\beta}G(i\nu_n)^{-2}$, where \underline{K} is the Jacobian

$$K_{ln}^{\alpha\beta}=\frac{\delta G(i\nu_n)_{\beta\beta}}{\delta[G_0(i\nu_l)_{\alpha\alpha}]^{-1}}=-\delta_{ln}\frac{1}{a_n^2}\left\{\frac{2\tilde{J}_H^2}{3}+b_n\delta_{\alpha\beta}\right\}+\frac{\tilde{J}_H^2}{3a_n a_n}(2\delta_{\alpha\beta}-1), \quad (11)$$

with $a_n=G_0(i\nu_n)^{-2}-\tilde{J}_H^2$ and $b_n=G_0(i\nu_n)^{-2}-\tilde{J}_H^2/3$. This Jacobian can be inverted with the general result

$$\frac{\delta\Sigma(i\nu_l)_{\alpha\alpha}}{\delta G(i\nu_n)_{\beta\beta}}=-\delta_{ln}\frac{\tilde{J}_H^2 a_n^2}{3b_n}\left\{\frac{2}{2a_n-3b_n}+\delta_{\alpha\beta}G_0(i\nu_n)^2\right\}-\frac{\tilde{J}_H^2}{3-2\tilde{J}_H^2\sum_r 1/b_r} \frac{a_l a_n}{b_l b_n}(2\delta_{\alpha\beta}-1). \quad (12)$$

It can be shown¹⁴ that the right-hand side equals $-T\Gamma(l,n;m=0)^{\alpha\alpha;\beta\beta}$ where $\Gamma(l,n;m)^{\beta\alpha;\delta\kappa}$ is the full irreducible vertex of the Bethe-Salpeter equation. The functional Φ must exist because the curl of the self-energy vanishes: $\delta\Sigma(i\nu_n)_{\alpha\alpha}/\delta G(i\nu_l)_{\beta\beta}-\delta\Sigma(i\nu_l)_{\beta\beta}/\delta G(i\nu_n)_{\alpha\alpha}=0$.

By construction, $\Phi^{(1)}$ (second order in J_H) is represented by the compact diagram in Fig. 1(b) and is given in terms of the bare vertex function by

$$\Phi^{(1)}=-\frac{T}{2}\sum_{l,r}\Gamma^{(0)}(l,r;0)^{\alpha\alpha;\beta\beta}G(i\nu_l)_{\alpha\alpha}G(i\nu_r)_{\beta\beta}=-\frac{\tilde{J}_H^2}{6}\left\{\sum_{l,n}G(i\nu_l)_{\alpha\alpha}(G(i\nu_n)_{\alpha\alpha}-G(i\nu_n)_{\bar{\alpha}\bar{\alpha}})-\sum_n G(i\nu_n)_{\alpha\alpha}^2-2\sum_n G(i\nu_n)_{\alpha\alpha}G(i\nu_n)_{\bar{\alpha}\bar{\alpha}}\right\}, \quad (13)$$

where $\bar{\alpha}$ is the opposite spin to α . After expanding and integrating Eq. (12),¹⁹ we find that $\Phi^{(2)}$ (fourth order in J_H) is given by

$$\Phi^{(2)}=\frac{\tilde{J}_H^4}{9}\left\{-\frac{1}{4}\sum_n G(i\nu_n)_{\alpha\alpha}^4-2\sum_n G(i\nu_n)_{\alpha\alpha}^2 G(i\nu_n)_{\bar{\alpha}\bar{\alpha}}^2-\sum_{l,n,r} G(i\nu_r)_{\alpha\alpha}G(i\nu_r)_{\bar{\alpha}\bar{\alpha}}G(i\nu_l)_{\alpha\alpha}(G(i\nu_n)_{\alpha\alpha}-G(i\nu_n)_{\bar{\alpha}\bar{\alpha}})+\frac{2}{3}\sum_{l,n} G(i\nu_n)_{\alpha\alpha}^3(G(i\nu_l)_{\alpha\alpha}-G(i\nu_l)_{\bar{\alpha}\bar{\alpha}})\right\}. \quad (14)$$

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 $\mathbf{H}=\mathbf{H}z$ coupled to both the local moments and the electrons, the effective action becomes

$$A_{\text{eff}}(\mathbf{m})=-T\sum_n \bar{c}_{0\alpha}(i\nu_n)\left\{G_0(i\nu_n)_{\alpha\beta}^{-1}+\left(\tilde{J}_H\mathbf{m}+\frac{1}{2}\mathbf{H}z\right)\cdot\sigma_{\alpha\beta}\right\}\times c_{0\beta}(i\nu_n)-\beta H S m_z. \quad (15)$$

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 $G_0(i\nu_n)^{-1}=(z_n+R_n)\mathbf{I}+Q_n\sigma_z$ and using Eq. (5), we solve for R_n and Q_n from the expression

$$R_n\mathbf{I}+Q_n\sigma_z=-\frac{W^2}{16}\langle\{(z_n+R_n)\mathbf{I}+[\tilde{J}_H\mathbf{m}+(Q_n+H/2)\mathbf{z}]\cdot\sigma\}^{-1}\rangle_{\mathbf{m}}. \quad (16)$$

To linear order in the field, R_n and Q_n satisfy the implicit relations

$$R_n=-\frac{W^2}{16}\frac{z_n+R_n}{(z_n+R_n)^2-\tilde{J}_H^2}, \quad (17)$$

$$Q_n=\frac{H(z_n+R_n)-2\tilde{J}_H M_{\text{lm}} R_n}{2(z_n+2R_n)U_n}-\frac{H}{2}, \quad (18)$$

where

$$U_n=1-\frac{32\tilde{J}_H^2}{3W^2}\frac{R_n^2}{(z_n+R_n)(z_n+2R_n)}. \quad (19)$$

After integrating $\exp(-A_{\text{eff}}(\mathbf{m}))$ over the Grassman variables, we find that the probability for the local moment to point along \mathbf{m} is

$$P(\mathbf{m})\propto\exp\left\{\sum_n \ln\left(1-\frac{\tilde{J}_H(2Q_n+H)m_z}{(z_n+R_n)^2-\tilde{J}_H^2}\right)+\beta H S m_z\right\}\propto\exp(\beta J_{\text{eff}} M_{\text{lm}} m_z). \quad (20)$$

The last relation is written to lowest order in the local-moment order parameter $M_{\text{lm}}=\langle m_z \rangle_{\mathbf{m}}$ and defines the effective interaction

$$J_{\text{eff}}=\frac{16T\tilde{J}_H}{W^2}\sum_n \frac{R_n}{(z_n+R_n)(z_n+2R_n)U_n}\left\{\chi_{\text{lm}}^{-1}(z_n+R_n)-2\tilde{J}_H R_n\right\}+\chi_{\text{lm}}^{-1}S, \quad (21)$$

where $\chi_{\text{lm}}=M_{\text{lm}}/H$ is the local-moment susceptibility. Now M_{lm} is solved from the condition $M_{\text{lm}}=J_{\text{eff}}M_{\text{lm}}\beta/3$, which contains terms proportional to both H and M_{lm} on the right-hand side. The electronic order parameter $M_{\text{el}}=2\langle s_{0z} \rangle$ is obtained from the summation $M_{\text{el}}=-(32T/W^2)\sum_n Q_n$. The total-spin susceptibility is then given by the zero-field limit of $\chi=(SM_{\text{lm}}+M_{\text{el}}/2)/H$.

To calculate the susceptibility from the partition function, we first expand Z to the second order in H and M_{lm} and then use $\chi=(T/H)\partial \ln Z/\partial H|_{H=0}$. 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

$$\chi = \frac{1}{3T} \frac{S_{\text{eff}}(T)^2}{1 - (\tilde{J}_H/W)^2 G_1(T)} + \frac{3T}{4W^2} (G_1(T) - G_2(T)) + \frac{8\tilde{J}_H^2 T}{W^4} G_1(T), \quad (22)$$

$$S_{\text{eff}}(T) = S + \frac{3\tilde{J}_H T}{2W^2} (G_1(T) - G_2(T)), \quad (23)$$

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

$$G_1(T) = -\frac{32}{3} \sum_n \frac{R_n^2}{(z_n + R_n)(z_n + 2R_n)U_n}, \quad (24)$$

$$G_2(T) = -\frac{32}{3} \sum_n \frac{R_n}{(z_n + R_n)U_n}. \quad (25)$$

The Curie temperature T_C is solved from the condition $G_1(T_C) = (W/\tilde{J}_H)^2$. 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.

Previous results⁸ in the $J_H \rightarrow \infty$ limit are reproduced²⁰ by taking $\mu = \text{sgn}(p-1)\tilde{J}_H + \delta\mu$ where $|\delta\mu| \leq W/(2\sqrt{2})$ and p is the electron filling ($p=1$ means one electron per site). The general expression for the magnetic susceptibility shall be studied in a future publication. We pause here to note that the effective spin $S_{\text{eff}}(T)$ may be either larger or smaller than S depending on the sign of the Hund's coupling J_H . The tem-

perature dependence of $S_{\text{eff}}(T)$ and the deviation of $1 - (\tilde{J}_H/W)^2 G_1(T)$ from $T - T_C$ are both caused by electronic correlations that are absent in a local-moment system.⁸ The second and third sets of terms in Eq. (22) correspond to the Pauli susceptibility of the electrons.

Although $\Phi(\{G(i\nu_n)\})$ has no simple diagrammatic expansion in terms of the bare vertex function and the full Green's function, the existence of this functional means that Eq. (10) may still be used to establish the general 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 Kadanoff¹⁶) 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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¹⁹Due to the term containing $\{1 - (2/3)\tilde{J}_H^2 \sum_i (G_0(i\nu_i))^{-2} - \tilde{J}_H^2/3\}^{-1}$ in the irreducible vertex function Γ , the radius of convergence of the expansion in powers of \tilde{J}_H is of order T . In the limit $J_H \rightarrow \infty$, Γ depends on the cutoff n_χ of the Matsubara sum (Ref. 8).

²⁰In the $J_H \rightarrow \infty$ limit, $G_1(T) \rightarrow (W/\tilde{J}_H)^2 F_1(T)$ and $G_2(T) \rightarrow (W^2/3\tilde{J}_H T)\{|p-1| - 1 - 2 \text{sgn}(p-1)F_2(T)\}$, where $F_1(T)$ and $F_2(T)$ were defined in Ref 8.