Magnetic Susceptibility and Order Parameter of the Spin-Glass-Like Phase of the Double-Exchange Model

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The magnetic susceptibility and Edwards-Anderson order parameter q of the spin-glass-like (SGL) phase of the double-exchange model are evaluated in the weak-coupling or RKKY limit. Dynamical mean-field theory is used to show that $q = M(T/T_{\mathrm{SGL}})^2$, where M is the classical Brillouin function and T_{SGL} is the SGL transition temperature. The correlation length of the SGL phase is determined by a correlation parameter Q that maximizes T_{SGL} and minimizes the free energy. The magnetic susceptibility has a cusp at T_{SGL} and reaches a nonzero value as $T \to 0$.

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Models that exhibit spin-glass-like (SGL) behavior for classical spins in the absence of quenched disorder have attracted a great deal of theoretical attention [1] since the experimental discovery of spin ice [2] in rare-earth pyrochlores. In geometrically frustrated magnets [3] like spin ice, ferromagnetic (FM) interactions are frustrated by constraints on the spin directions. Because these systems are not amenable to analytic calculations, they are typically studied using Monte Carlo techniques [4]. In this Letter, we examine the SGL phase of a very different model that, like spin ice, contains no quenched disorder. Analytic results are now obtained for the SGL phase of a model with classical spins but without geometric frustration.

One of the most important models of itinerant systems, the double-exchange (DE) model is believed to describe many physical systems ranging from the manganites [5] to dilute magnetic semiconductors [6]. In the weak-coupling limit, the DE model becomes equivalent [7] to a RKKY model with competing antiferromagnetic (AF) and FM Heisenberg interactions between classical spins at every site. In a typical spin glass, such as CuMn [8], the RKKY interactions between randomly alloyed Mn ions produce a disordered ground state with a massive degeneracy. Recent work [9] on the DE model has revealed that the competing RKKY interactions between magnetic moments on a Bethe lattice can stabilize a phase with short-range but not long-range magnetic order [10]. We now show that the magnetic susceptibility of this SGL phase has a cusp at T_{SGL}, marking the onset of short-range order, and reaches a nonzero value as $T \to 0$. The Edwards-Anderson (EA) order parameter q [12,13] of the SGL phase is identical to the square of the classical Brillouin function $M(T/T_{\mathrm{SGL}})$.

The DE model contains a kinetic term that describes the hopping of electrons between neighboring sites and a potential term that aligns the electronic spins with the classical local moments at every site. There is no quenched disorder in the DE Hamiltonian (also called the FM Kondo Hamiltonian when the coupling is finite)

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

where $c^{\dagger}_{i\alpha}$ and $c_{i\alpha}$ are the creation and destruction operators for an electron with spin α at location $\mathbf{R}_i$, $\mathbf{s}_i = c^{\dagger}_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}/2$ is the electronic spin, and $\mathbf{S}_i = S\mathbf{m}_i$ is the classical spin of the local moment. Repeated spin indices are summed. When $J_H > 0$, Hund's coupling favors the alignment of the local moments with the electronic spins. Because of the electron-hole symmetry of the DE model, we shall only consider electron concentrations p between 0 and 1 carriers per site. For small p, the hopping of electrons between neighboring sites favors the alignment of the local moments and the FM phase is stable. Since electrons with parallel spins cannot hop between singly occupied sites due to the Pauli exclusion principle, the AF phase is favored over the FM phase near $p = 1$. But as shown in Ref. [9] using dynamical mean-field theory (DMFT), the competing FM and AF interactions may actually favor a SGL phase over the ordered phases for small J_H.

Developed in the late 1980's by Müller-Hartmann [14] and Metzner and Vollhardt [15], DMFT exploits the momentum independence of the electronic self-energy in infinite dimensions. Even in three dimensions, DMFT is believed to capture the physics of correlated systems including the narrowing of electronic bands and the Mott-Hubbard transition [16]. Within DMFT, the local effective action on any site is parameterized by a Green's function that regulates the hopping of correlated electrons from other sites. We will use DMFT to study the DE model on a Bethe lattice in infinite dimensions. The bare density-of-states of a Bethe lattice with $z \gg 1$ nearest neighbors is $N_0(\mu) = (4/\pi W)\sqrt{1-(2\mu/W)^2}$, where $W = 4\sqrt{z}t$ is the bandwidth and μ is the chemical potential. Since the Bethe lattice is *not* translationally invariant, $\mathbf{q} = 0$ is the only well-defined wave vector [9].

In infinite dimensions, the high-temperature nonmagnetic (NM) phases of the Heisenberg and DE models have a vanishing correlation length ξ. The SGL phase is a bulk solution of the DE model with some of the same characteristics as conventional spin glasses: a finite local magnetization and spin-spin correlations that decay exponentially over distance [8]. The SGL phase is characterized

by a correlation parameter Q, defined as the average over all neighbors of $\sin^2(\theta_i/2)$, where θ_i is the angle between the central spin and a neighboring spin. Overall, the neighboring spins describe a cone with angle $2\arcsin(\sqrt{Q})$ around the central spin. The FM and AF phases have, respectively, $Q = 0$ and 1. The magnetization about every site decays exponentially with a correlation length $\xi = -a/\log|2Q - 1|$, where a is the lattice constant. Notice that ξ/a diverges in the FM and AF phases but vanishes in the NM state obtained by setting $Q = 1/2$. Mathematically, the SGL phase was first introduced by Chattopadhyay *et al.* [17], although its physical significance was not recognized until later. In lower dimensions, the SGL phase evolves into the phase with incommensurate correlations obtained in Monte Carlo simulations [18]. Detailed discussions of the $T = 0$ phase diagram and magnetic instabilities of the DE model, including the issue of phase separation, are contained in Ref. [9].

As shown earlier [9], the transition temperature $T_{\mathrm{SGL}}(p, Q)$ of the SGL phase may be evaluated from coupled Green's function equations. In the weak-coupling limit $J_H S \ll W$ and $T \sim (J_H S)^2/W$, $T_{\mathrm{SGL}}(p, Q)$ is implicitly given by the expression $T_{\mathrm{SGL}}(p, Q) = J_{\mathrm{eff}}(p, Q)/3$ where

$$J_{\mathrm{eff}}(p, Q) = -2(J_H S)^2(2Q - 1)T \times \sum_n \frac{R_n}{(z_n + R_n)^2(z_n + 2(1 - Q)R_n)}, \quad (2)$$

with $R_n = (-z_n + \sqrt{z_n^2 - W^2/4})/2$, $z_n = i\nu_n + \mu$, and $\nu_n = (2n + 1)\pi T$. Since $T \ll W$, the sum $T\sum_n F(\nu_n)$ is equivalent to the integral $(1/2\pi)\int d\upsilon F(\upsilon)$ and $J_{\mathrm{eff}}(p, Q)$ is independent of temperature. The relation $T_{\mathrm{SGL}}(p, Q) = J_{\mathrm{eff}}(p, Q)/3$ correctly reduces to the FM ($Q = 0$) result first derived in Refs. [19,20]. Another derivation of $T_{\mathrm{SGL}}(p, Q)$ was recently provided in Ref. [21]. Of course, $T_{\mathrm{SGL}}(p, Q)$ vanishes in the NM state with $Q = 1/2$.

After $T_{\mathrm{SGL}}(p, Q)$ is maximized with respect to Q, $T_{\mathrm{SGL}}(p)$ exceeds the Curie and Néel temperatures in the concentration range $0.26 < p < 1$. The correlation parameter Q changes discontinuously at $T_{\mathrm{SGL}}(p)$ from $1/2$ in the NM phase above to a value less than or greater than $1/2$ in the SGL phase below. The ground state is NM with $Q = 1/2$ for a single concentration close to $p = 0.5$.

The temperature dependence of the local SGL order parameter $M = |\langle \mathbf{m}_i \rangle|$ on site i may be evaluated in a local environment fixed by the correlation parameter Q by integrating the local action over the Fermion variables. The probability for $\mathbf{m}_i$ to point at an angle $\cos\theta$ with respect to the local quantization axis is proportional to $\exp(MJ_{\mathrm{eff}}\beta\cos\theta) = \exp((3M\cos\theta)/\tau)$, where $\tau = T/T_{\mathrm{SGL}}$. Consequently, M has the solution

$$M(\tau) = \coth\left(\frac{3M}{\tau}\right) - \frac{\tau}{3M}, \quad (3)$$

which is just the Brillouin function in the $S \to \infty$ or classical limit [11], plotted in Fig. 1. The result for the FM order parameter (taking $Q = 0$ and $T_{\mathrm{SGL}} = T_C$) is not surprising considering the weak-coupling equivalence between the DE model and a Heisenberg model with RKKY interactions between classical spins. What is surprising is that with a simple change in critical temperature, the short-range order parameter of the SGL phase is identical to the long-range order parameter of the FM phase. For small τ, $M(\tau) \approx 1 - \tau/3 - \tau^2/9 + \vartheta(\tau^3)$.

To zeroth order in $J_H S/W$, p is given in terms of μ by $p = 1/2 + (1/\pi)\{\delta\sqrt{1 - \delta^2} + \sin^{-1}\delta\}$, where $\delta = 2\mu/W$. Carefully accounting for the dependence of the chemical potential $\mu(p)$ on $J_H S/W$ for a fixed p, we have generalized the $T = 0$ relation derived in Ref. [9] for the energy difference $\Delta E(p, Q)$ between the SGL and NM phases: $\Delta E(p, Q)/N = -(3/2)M(\tau)^2 T_{\mathrm{SGL}}(p, Q)$, where both sides are evaluated analytically to order $(J_H S)^2/W$. This relation is precisely the same as the MF result for the FM phase of a classical Heisenberg model. By integrating the specific heat to obtain the entropy, we have formally constructed the free energy difference $\Delta F(p, Q)$ [22] between the SGL and NM phases. Because $(1/N)\partial\Delta F/\partial Q = -(3/2)M(\tau)^2\partial T_{\mathrm{SGL}}/\partial Q$, the free energy is minimized by the same correlation parameter Q that maximizes the transition temperature.

We now evaluate the magnetic susceptibility of the FM and SGL phases in the weak-coupling limit by utilizing the formalism developed by Fishman and Jarrell [23]. Treating the electronic susceptibility as a $2n_\chi$-dimensional matrix, the local-moment susceptibility as a scalar, and the cross terms as $2n_\chi$-dimensional vectors in Matsubara space, $\underline{\chi}(\mathbf{q} = 0, i\omega_m)$ can be written as a $(2n_\chi + 1) \times (2n_\chi + 1)$ supermatrix. The total susceptibility $\chi(\mathbf{q} = 0, i\omega_m)$ is obtained by taking $n_\chi \to \infty$ and summing $\underline{\chi}(\mathbf{q} = 0, i\omega_m)$

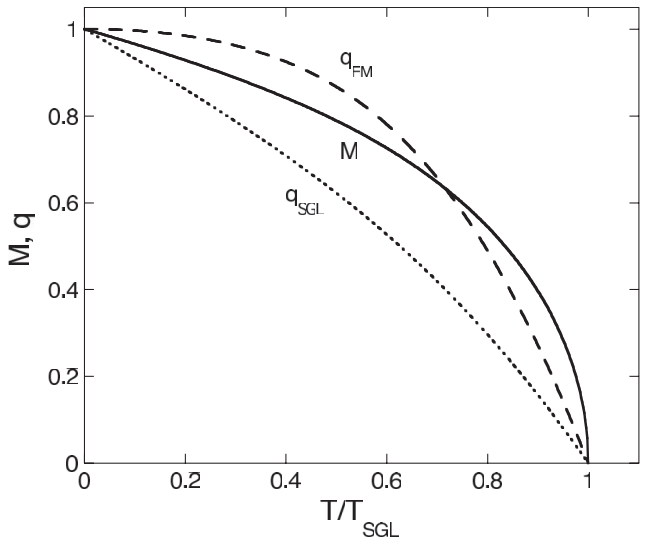

FIG. 1. The Brillouin function $M(\tau)$ and EA order parameters $q(\tau)$ versus $\tau = T/T_{\mathrm{SGL}}$.

over all matrix elements for a fixed external frequency $\omega_m = 2m\pi T$. As discussed in Ref. [23], $\underline{\chi}(\mathbf{q} = 0, i\omega_m)$ satisfies the Bethe-Salpeter equation

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

where $\underline{\Gamma}(i\omega_m)$ is the vertex function and $\underline{\chi}^{(0)}(\mathbf{q} = 0, i\omega_m)$ is the bare susceptibility. 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, $\underline{\Gamma}(i\omega_m)$ is independent of momenta and may be evaluated from an identical Bethe-Salpeter equation where $\underline{\chi}(\mathbf{q} = 0, i\omega_m)$ and $\underline{\chi}^{(0)}(\mathbf{q} = 0, i\omega_m)$ are replaced by local susceptibilities at a site i. Because the total spin $\sum_i(\mathbf{S}_i + \mathbf{s}_i)$ is conserved, the $\mathbf{q} = 0$ susceptibility $\chi(\mathbf{q} = 0, i\omega_m)$ is proportional to $\delta_{m,0}$. So we shall henceforth take $\omega_m = 0$ to evaluate the elastic susceptibility $\chi(\mathbf{q} = 0)$.

The magnetic field is taken to lie along the magnetization direction in the FM phase but is averaged over all orientations in the SGL phase, which has no net magnetization. For example, the bare local-moment susceptibility on site i is given by $\beta S^2\{\langle m_{i\alpha}^2\rangle - \langle m_{i\alpha}\rangle^2\} \Rightarrow \beta S^2(1 - q)/3$, where $q = M^2$ in the SGL phase and $q = 3M^2 - 2(1 - T/T_C) > 0$ $(T < T_C)$ or 0 $(T > T_C)$ in the FM phase. Following the derivation in Ref. [23], we find that the total, elastic susceptibility is given by

$$\chi(\mathbf{q} = 0) = \frac{S_{\text{eff}}^2}{3}\frac{1 - q}{T - T_C(1 - q)} + \frac{N_0(\mu)}{2}, \quad (5)$$

where $S_{\text{eff}} = S + J_H S N_0(\mu)$. Since $N_0(\mu) \propto 1/W$, the electronic contribution $J_H S N_0(\mu)$ is much less than the local-moment contribution S to S_{eff} in the weak-coupling limit [24]. The electronic contribution enlarges or diminishes S_{eff} depending on the sign of J_H. The final term in Eq. (5), $N_0(\mu)/2$, is just the electronic Pauli susceptibility. Since it does not depend on J_H and exhibits only weak temperature dependence, we shall neglect the Pauli susceptibility in the subsequent discussion. For a FM, the Curie-Wess susceptibility of Eq. (5) with $S_{\text{eff}} = S$ is precisely the same as the MF result for a classical Heisenberg model [11]. Bare in mind that the broad analogies between the (D)MF theories of the DE and classical Heisenberg models only exist in the weak-coupling limit and disappear once $J_H S$ becomes of order W. In the strong-coupling limit $J_H S \gg W$, the magnetic susceptibility is more complex than Eq. (5) with a Curie constant that deviates from $S^2/3$ in the large S limit [23].

Using the low-temperature behavior of $M(\tau)$, we find that $q_{\text{FM}} \to 1 - \tau^2/3$ and $\chi(\mathbf{q} = 0) \to (S_{\text{eff}}^2/9)T/T_C^2$ as $T \to 0$ in the FM phase. By contrast, $q_{\text{SGL}} \to 1 - 2\tau/3$ and $\chi(\mathbf{q} = 0) \to (S_{\text{eff}}^2/3)/(3T_{\text{SGL}}/2 - T_C)$ as $T \to 0$ in the SGL phase. Because the SGL phase has no long-range order and the local moments have no preferred orientation for any Q between 0 and 1, the zero-temperature susceptibility does not vanish as $p \to 0.26$ and $T_{\text{SGL}} \to T_C$. The magnetic susceptibility in the SGL phase is plotted versus τ for several different concentrations in Fig. 2. As expected, the SGL susceptibility has a cusp at T_{SGL}, which develops into a divergence as $p \to 0.26$ and $Q \to 0$. Notice that the normalized susceptibility $T_{\text{SGL}}\chi(\mathbf{q} = 0)/S_{\text{eff}}^2$ vanishes as $Q \to 1/2$ and $T_{\text{SGL}} \to 0$ in the vicinity of $p = 0.5$.

Comparing Eq. (5) with the parameterization of Sherrington and Kirkpatrick (SK) [13], we conclude that q is the EA order parameter [12]. We have plotted q_{SGL} and q_{FM} versus τ in Fig. 1. Our result $q_{\text{SGL}} = \langle \mathbf{m}_i\rangle^2$ should be compared with the SK expression $q = \langle\langle S_i\rangle^2\rangle_J$, where the inner expectation value is a thermal average for a given set of exchange couplings and the outer is an ensemble average over the distribution of exchange couplings. For the DE model, the EA order parameter is the same at every site even without an average over quenched disorder. The DMFT result for the DE model differs from the SK result for the random $S = 1/2$ Ising model in at least one important respect: the SK prediction for $\sqrt{q}$ is *not* identical to the $S = 1/2$ Brillouin function whereas $\sqrt{q_{\text{SGL}}}$ is equivalent to the $S = \infty$ Brillouin function. Our result for q_{SGL} is qualitatively similar to the EA order parameter of spin ice, evaluated with Monte Carlo simulations [4].

To summarize, we have calculated the total, magnetic susceptibility and EA order parameters of the SGL phase in the weak-coupling or RKKY limit. We find that the SGL susceptibility has a cusp at T_{SGL} and reaches a nonzero constant as $T \to 0$, as expected for a phase with only short-range magnetic order. The SGL phase is characterized by the absence of long-range order in $\langle \mathbf{m}_i\rangle$ but by the nonzero value of $\langle \mathbf{m}_i\rangle^2$. These were the original SK criteria [13] for the existence of a spin glass. Unlike the spin glass ground state of the random Ising model or the SGL ground state of spin ice, the SGL phase of the DE model can be studied analytically in the absence of quenched disorder and without geometric frustration.

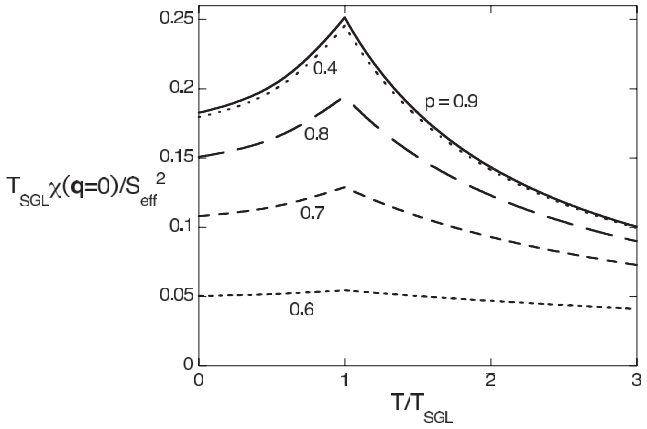

FIG. 2. The elastic, $\mathbf{q} = 0$ susceptibility versus T/T_{SGL} for several electron concentrations p.

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