Critical and Griffiths-McCoy singularities in quantum Ising spin glasses on d-dimensional hypercubic lattices: A series expansion study

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We study the $\pm J$ transverse-field Ising spin-glass model at zero temperature on d-dimensional hypercubic lattices and in the Sherrington-Kirkpatrick (SK) model, by series expansions around the strong-field limit. In the SK model and in high dimensions our calculated critical properties are in excellent agreement with the exact mean-field results, surprisingly even down to dimension $d = 6$, which is below the upper critical dimension of $d = 8$. In contrast, at lower dimensions we find a rich singular behavior consisting of critical and Griffiths-McCoy singularities. The divergence of the equal-time structure factor allows us to locate the critical coupling where the correlation length diverges, implying the onset of a thermodynamic phase transition. We find that the spin-glass susceptibility as well as various power moments of the local susceptibility become singular in the paramagnetic phase *before* the critical point. Griffiths-McCoy singularities are very strong in two dimensions but decrease rapidly as the dimension increases. We present evidence that high enough powers of the local susceptibility may become singular at the pure-system critical point.

The combination of quantum mechanics and disorder leads to rich behavior at and near zero-temperature quantum critical points (QCPs). For example, the one-dimensional random transverse-field Ising model has a QCP in which the average and typical correlation functions have different critical exponents [1,2] and the time dependence is described by activated dynamical scaling, in which the log of the relaxation time is proportional to a power of the correlation length ξ, rather than conventional dynamical scaling, in which the relaxation time itself is proportional to ξ^z, where z is the dynamical exponent. Distributions of several quantities are very broad at the QCP so QCPs with these features are said to be of the "infinite-randomness" type. It has been proposed [3] that infinite-randomness QCPs can occur at dimensions higher than 1. It is also proposed [3] that the infinite-randomness QCP can occur in spin glasses, on the grounds that frustration is irrelevant since the distribution of renormalized interactions (as one performs renormalization-group transformations) is so broad that only the largest one matters.

In addition, singularities can occur in the paramagnetic phase in the region where the corresponding *nonrandom* system would be ordered. This was first pointed out for classical systems by Griffiths [4], though the singularities turn out to be unobservably weak in that case [5]. However, these singularities are much stronger in the quantum case, as first shown by McCoy [6,7], and can lead to power-law singularities in *local* quantities in part of the paramagnetic phase. For quantum problems we refer to these effects as Griffiths-McCoy (GM) singularities. For a review see Ref. [8], and for recent experimental observations of GM singularities see Ref. [9]. In the quantum paramagnetic phase in the limit as $T \to 0$ GM singularities are characterized by a dynamical

exponent z' which varies as the QCP is approached. For infinite-randomness QCPs, $z' \to \infty$ as the QCP is approached [3,8].

In this paper we study the QCP and GM singularities in quantum spin glasses. The infinite-range version, the Sherrington-Kirkpatrick (SK) model [10] in a transverse field, has been studied in detail [11–13], and the mean-field behavior determined. There have also been quantum Monte Carlo (QMC) studies in dimension $d = 2$ [14] and $d = 3$ [15]. In this paper we study quantum spin glasses using series expansions at $T = 0$, in which we expand away from the high transverse-field limit. We feel that the series expansion method is complementary to QMC simulations and has certain advantages: (i) we study the *whole range* of dimensions from $d = 2$ to the SK model (which is effectively infinite d), (ii) we work at strictly zero temperature, whereas in the QMC one has to extrapolate to $T = 0$ using a rather complicated anisotropic finite-size scaling procedure [14,15], and (iii) averaging over bond disorder is done exactly. As in the QMC we can see GM singularities (we think our work is the first time these singularities have been seen using series methods) and, also, go beyond simple averages of local quantities, in our case by computing moments up to high order.

Our main conclusions are as follows. We show systematically how the strength of GM singularities diminishes rapidly as the dimension increases above 2, vanishing, as expected, for the SK model. In two dimensions, where GM singularities are strongest, our results make plausible the expectation that GM singularities persist in the paramagnetic phase all the way to the critical point of the pure system. We find that critical behavior close to that of mean-field theory persists *below* the upper critical dimension, $d_u = 8$ [13], down to $d = 6$, which is surprising since the renormalization group finds no perturbative fixed point below $d = 8$ [13]. Our results in two and three dimensions agree very well with earlier work [14,15].

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We consider the Hamiltonian

$$\mathcal{H} = -h^T \sum_{i=1}^{N} \sigma_i^x - \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z, \qquad (1)$$

where the σ_i^α are Pauli spin operators and h^T is the transverse field. The interactions J_{ij} are *quenched* random variables with a bimodal distribution. The N spins either lie on a hypercubic lattice, in which case the interactions are between nearest neighbors and take values $\pm J$ with equal probability, or correspond to the SK [10] model, in which case there is no lattice structure, every spin interacts with every other spin, and $J_{ij} = \pm J/\sqrt{N}$. We choose a bimodal distribution because the series can be worked out much more efficiently for this case than for a general distribution [16]. We also add longitudinal fields h_i, as well as coupling to σ_i^z to define the spin-glass susceptibility, and set them to 0 afterwards [see Eqs. (3) and (4) below].

The zero-temperature quantities we calculate are as follows.

(a) The zero-wave-vector, equal-time structure factor defined as

$$S(0) = \frac{1}{N} \sum_{i,j} \left[\langle 0|\sigma_i^z \sigma_j^z|0\rangle^2 \right]_{\mathrm{av}}, \qquad (2)$$

where state $|0\rangle$ is the ground state of the system, and the average $[\cdot]_{\mathrm{av}}$ refers to the disorder average over the quenched random bonds.

(b) The spin-glass susceptibility, defined as

$$\chi_{\mathrm{SG}} = \frac{1}{N} \sum_{i,j} \left[\chi_{ij}^2 \right]_{\mathrm{av}}, \qquad (3)$$

where the ground-state energy $E(\{h_i\})$ in the presence of infinitesimal longitudinal fields h_i defines the local susceptibilities χ_{ij} by the relation

$$E(\{h_i\}) = E_0 - \frac{1}{2} \sum_{i,j} \chi_{ij} \, h_i h_j. \qquad (4)$$

(c) The moments of the local susceptibility, defined as

$$\chi_m = \frac{1}{N} \sum_i \left[\chi_{ii}^m \right]_{\mathrm{av}}. \qquad (5)$$

We use the linked cluster method to generate the series [19] and discuss the details of the computational method elsewhere [16]. We expand away from the trivial paramagnetic state with $J = 0$, so the expansion parameter is

$$x = (J/h^T)^2. \qquad (6)$$

The series are obtained to order 14 for the SK model and for $d = 2$ and 3 and to order 10 in higher dimensions. The series coefficients can be found in the Supplemental Material [20]. Throughout this paper we generically refer to the coefficients of the series expansions as a_n, meaning that the series is of the form

$$Q = \sum_n a_n x^n. \qquad (7)$$

We find that, in contrast to classical spin glasses [21,22], the series for the quantum systems are surprisingly well behaved.

Most of our analysis is based on the simple ratio method, although we have checked that d-log Pade analysis gives answers consistent with them. If the series has a simple power-law variation, $Q \propto (x - x_c)^{-\lambda}$, then the ratios satisfy

$$r_n \equiv \frac{a_n}{a_{n-1}} = \frac{1}{x_c} \left(1 + \frac{\lambda - 1}{n} \right). \qquad (8)$$

Hence, in a plot of the ratio r_n versus $1/n$, the intercept gives $1/x_c$ and the slope for $1/n \to 0$ gives $(\lambda - 1)/x_c$. We do linear and quadratic fits to our data to extract x_c and the exponent.

Griffiths-McCoy singularities occur in a quantum disordered system at low T in the region between the critical point of the system and the critical point of the corresponding pure system. In this range, there are regions of the sample which are nondisordered and so are "locally in the ordered, symmetry-broken state." The very slow tunneling between the symmetry-broken states leads to power-law singularities [8,23–25] in the paramagnetic phase, coming from purely local physics, namely, a distribution of local relaxation times which extends up to very high values.

TABLE I. Estimates of points of singularity and exponents in various dimensions and the SK model. Note that $1/x_c \equiv (h_c^T/J)^2$. We anticipate that the singularity found for the equal time structure factor $S(0)$ is the critical singularity and so has exponent $\gamma - 2z\nu$. If the QCP is of the infinite-randomness type, then z and γ are infinite but the combination $\gamma - 2z\nu$ is presumably finite. For χ_{SG} the critical exponent is γ, but for low dimensions the susceptibility singularity is clearly at a larger value of $1/x_c$ than the critical singularity determined from $S(0)$, i.e., it is in the paramagnetic phase. Consequently, the series is finding a GM singularity for χ_{SG} rather than the critical singularity, so we denote the exponent by λ rather than γ. For the SK model GM singularities do not occur, so $\lambda = \gamma$ and the exact values are $\gamma = 1/2$, $\gamma - 2z\nu = -1/2$ [11–13], with logarithmic corrections for χ_{SG} as discussed in the text. The value of $(h_c^T/J)^2$ is estimated to be 2.268 in Ref. [17] and 2.28 ± 0.03 in Ref. [18]. In $d = 6$ and 8, GM singularities are very weak, and since the two values of x_c are almost the same, we expect that the series for χ_{SG} gives the critical singularity in these cases too. For the SK model, and for $d = 6$ and 8, we show results for χ_{SG} both with and without the mean-field log correction. No log correction is applied to $S(0)$ so the results for this quantity are the same in both rows. It is curious that the difference between the exponents for χ_{SG} and $S(0)$ is close to 1 for all models studied.

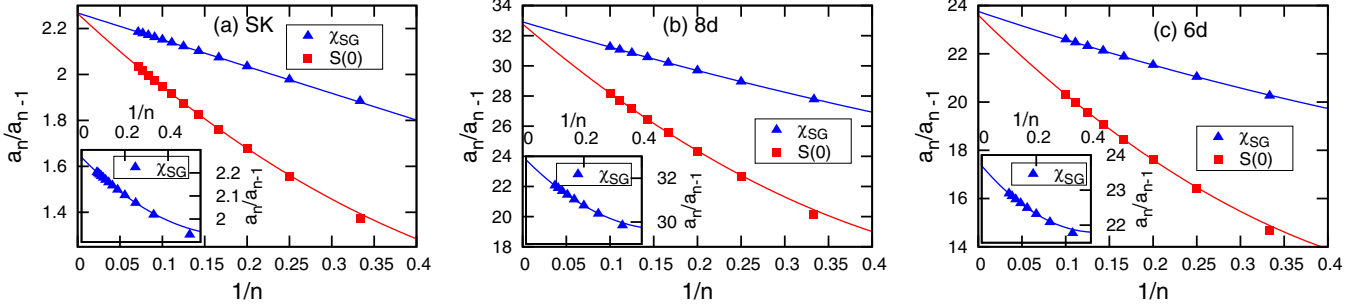| Model	χ_{SG}		$S(0)$	
	$1/x_c$	λ	$1/x_c$	$\gamma - 2z\nu$
SK	2.267	0.578	2.265	−0.509
SK (log)	2.268	0.486	2.265	−0.509
SK [11–13,17]	2.268	1/2	2.268	−1/2
SK [18]	2.28(3)		2.28(3)	
8d (log)	32.92	0.475	32.77	−0.515
8d	32.83	0.606	32.77	−0.515
6d (log)	23.75	0.489	23.60	−0.513
6d	23.68	0.628	23.60	−0.513
4d	14.46	0.697	14.23	−0.441
3d	9.791	0.796	9.411	−0.300
2d	5.045	1.281	4.521	0.284

FIG. 1. Ratio plots for (a) the SK model, (b) $d = 8$, and (c) $d = 6$. In all cases the differences in the intercept, i.e., the values of $1/x_c$, between results for $S(0)$ and results for χ_{SG}, is very small or 0, indicating that GM singularities are very small or nonexistent. Thus it is plausible that the singularity exponent for χ_{SG} is the *critical* exponent γ for these figures. The fits are quadratic except for χ_{SG} for the SK model, where we used a linear fit. The parameters of the fits are listed in Table I. In (a)–(c), the series for χ_{SG} had the mean-field log factor [11–13] incorporated. Insets: Ratios for χ_{SG} series *without* the log factor. The greater curvature is apparent.

Since χ_{SG} is the divergent response function for this problem, its *critical* exponent is defined to be [13] γ, i.e.,

$$\chi_{SG} \propto (x_c - x)^{-\gamma}. \tag{9}$$

However, it is important to stress that, because of GM singularities, the exponent determined in the series is usually different from γ, and we generally call it λ (see Table I). The equal-time structure factor $S(0)$ does not have the two time integrals present in χ_{SG}. Since the dynamic exponent is z and the correlation exponent is ν, the critical behavior of $S(0)$ is

$$S(0) \propto (x_c - x)^{-(\gamma - 2z\nu)}. \tag{10}$$

Because there are no time integrals in $S(0)$ we expect that GM singularities will not occur for this quantity, and any classical-like Griffiths [4] singularities will be unobservably weak [5]. If the QCP is of the infinite-randomness type, then γ and z will be infinite, though presumably the combination $\gamma - 2z\nu$ will be finite since it describes the critical behavior of the *equal-time* quantity $S(0)$.

We now discuss our results. Figures 1 and 2 show the ratios r_n for each model. The reader should also refer to Table I for values of the points of singularity and exponents.

We begin with the results for the SK model shown in Fig. 1(a). The critical point obtained, $1/x_c = 2.268$, is in excellent agreement with other studies [17,18]. The analytic prediction [11–13] is $\gamma = 1/2$ with a log correction. To

account for the log, we divide the series by $[-(1/t)\log(1 - t)]^{1/2}$, where $t = x/x_c$. Ratios of the resulting series give $\gamma = 0.49$, in excellent agreement with the exact result. Without taking logarithms into account, the exponent γ is estimated too high, at 0.58. Other predictions are [13] $z = 2$, $\nu = 1/4$, so $\gamma - 2z\nu = -1/2$ [the exponent for $S(0)$]. Our result for this is -0.51, again in good agreement. The critical points for χ_{SG} and $S(0)$ agree with each other to a high precision, indicating that there are no GM singularities in the SK mode, as expected.

Results of the ratio analysis of the series in $d = 8$ and $d = 6$ are shown in Figs. 1(b) and 1(c). Curiously the results for χ_{SG} work better, in the sense that the ratio plot is closer to a straight line, if one includes the *same* mean-field log correction as for the SK model. Of course, even if there are log corrections there is no *a priori* reason to assume that they have the same form as in mean-field theory. Including this correction the exponent for χ_{SG} is very close to the mean-field value of $1/2$. The exponent for $S(0)$ (for which no log correction is performed) is also close to the mean-field prediction of $-1/2$. There is very little difference in the critical points for χ_{SG} and $S(0)$, indicating that GM singularities, if present, are very weak. It is surprising that the same near-mean-field-like behavior is found in $d = 6$ as well as $d = 8$ since $d = 8$ is the upper critical dimension for this problem and no perturbative fixed point is found [13] below $d = 8$. One might therefore expect a dramatic change in critical behavior upon going below $d = 8$, but this is not what we find.
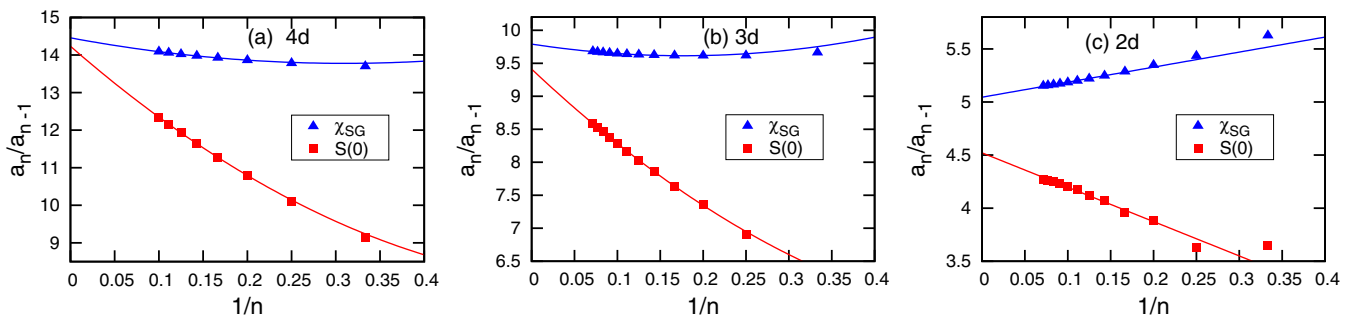

FIG. 2. Ratio plots for (a) $d = 4$, (b) $d = 3$, and (c) $d = 2$. In all cases there is a difference in the intercept, i.e., the value of $1/x_c$, between results for $S(0)$ and results for χ_{SG}, indicating that χ_{SG} diverges in the paramagnetic phase *before* the QCP is reached, i.e., the singularity in χ_{SG} corresponds to GM singularities, not critical singularities. Note that the difference in x_c values is very large in two dimensions but rapidly decreases with increasing dimension. The fits are linear for $d = 2$ and quadratic for $d = 3$ and 4. Parameters of the fits are listed in Table I.
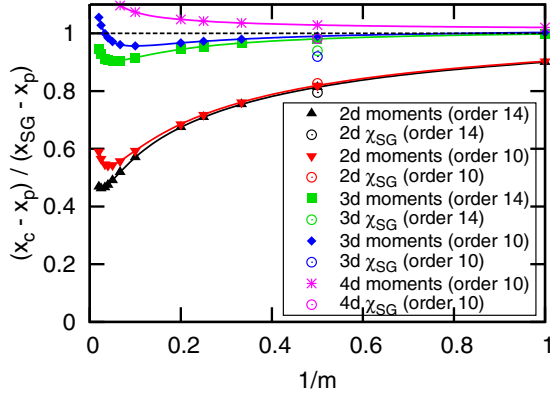
FIG. 3. Location of the singularity for the mth moment of the local susceptibility in $d = 2$, 3, and 4, plotted as a function of $1/m$. Here x_p is the critical point of the pure system, and x_{SG} is the spin-glass critical point as determined from the equal-time structure factor, so the y axis is scaled such that the pure-system critical point corresponds to $y = 0$ and the spin-glass critical point to $y = 1$. The spin-glass phase corresponds to $y > 1$, and the region of GM singularities to $0 < y < 1$.

In $d = 4$ [see Fig. 2(a)] there are clear deviations from mean-field exponents and a clear, though small, difference between the critical points for χ_{SG} and $S(0)$, indicating the presence of rather weak GM singularities. Comparing the results for $d = 4$ with those for $d = 3$ and 2 in Figs. 2(b) and 2(c), we see that the strength of GM singularities increases considerably with decreasing dimension. The same conclusion follows from comparing QMC results in $d = 3$ [24] with those in $d = 2$ [25]. For the critical singularity of $S(0)$ in $d = 3$ we find an exponent $\gamma - 2z\nu = -0.30$, which is in excellent agreement with the QMC calculations in Ref. [15], where -0.3 is obtained, which we deduce from their results $z \simeq 1.3$, $1/\nu \simeq 1.3$, $\eta + z \simeq 1.1$ [26] and the scaling relation $\gamma/\nu = 2 - \eta$. There is also good agreement in $d = 2$ between our value of 0.28 for the exponent for $S(0)$ and the QMC value [14] of 0.2 ± 0.1, which we deduce from their value of $(\gamma - 2z\nu)/\nu = 0.2 \pm 0.1$ in their Fig. 4 and $\nu = 1.0 \pm 0.1$.

We now study the GM singularities in more detail, focusing on the *local* susceptibility χ_{ii}. According to the standard picture [8,23–25], GM singularities occur because χ_{ii} is a random quantity, with a broad distribution extending out to very large values. Although we cannot compute the distribution of χ_{ii} directly we can get information on it indirectly by computing the series for moments of it, up to high order. The results are summarized in Fig. 3. The y axis is defined such that the critical value of x for the spin-glass problem is at $y = 1$ and the critical value for the pure ferromagnet (i.e., all interactions equal to J) is at $y = 0$.

Consider first the results in $d = 2$ shown in Fig. 3. We see that the higher moments have a singularity farther and farther away from the spin-glass critical point (which corresponds to $y = 1$). For large values of the order of the moment m, the 14th-order series lies below the 10th order series. It is therefore

plausible that, for an infinitely long series, the singularity approaches the pure-system critical point (i.e., $y = 0$) for $m \to \infty$.

Also shown in Fig. 3, by circles, are the locations of the divergence of the spin-glass susceptibility. This quantity has two time integrals and so we put these points at $m = 2$. In $d = 2$ the χ_{SG} singularities agree very well with the singularities in the local χ, confirming that the singularity found in χ_{SG} is a (local) GM singularity, not the critical singularity.

In $d = 3$, there seems to be a difference in Fig. 3 between the local χ and the χ_{SG} results, but note the opposite trends in the data between the 14-term and the 10-term series, so it is plausible that the two quantities would be singular at the same point in an infinitely long series.

In $d = 4$, the GM singularities are sufficiently weak that the local χ does not show a singularity at the QCP or in the paramagnetic phase, at least with a 10-term series. We expect that the singularity would be at the same location as that of χ_{SG} (which is just in the paramagnetic phase) for an infinitely long series.

To conclude, we have shown systematically how the strength of GM singularities diminishes rapidly as the dimension increases above 2, vanishing, as expected, for the SK model. In two dimensions, where GM singularities are strongest, our results make plausible the expectation that GM singularities persist in the paramagnetic phase all the way to the critical point of the pure system. We find that critical behavior close to that of mean-field theory persists *below* the upper critical dimension, $d_u = 8$ [13], down to $d = 6$, which is surprising since the renormalization group finds no perturbative fixed point below $d = 8$ [13]. Our results in two and three dimensions agree very well with earlier work [14,15].

Since the series for χ_{SG} sees GM singularities rather than critical singularities we cannot determine whether or not the QCP is of the infinite-randomness type (for which γ and z are infinite, though $\gamma - 2z\nu$ is finite). Recent numerical simulations in two dimensions [27] are argued to support the infinite-randomness scenario, though it seems to us that conventional critical behavior fits the data about as well. As the dimension increases, the effects of GM singularities become much weaker than in $d = 2$, so we conclude that if the infinite-randomness scenario occurs at all for $d > 2$, it must manifest itself only over a very small region around the quantum critical point.

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