Quantum-criticality and percolation in dimer-diluted 2D antiferromagnets

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The $S = 1/2$ Heisenberg model is considered on bilayer and single-layer square lattices with couplings $J_1$, $J_2$, and with each spin belonging to one $J_2$-coupled dimer. A transition from a Néel to disordered ground state occurs at a critical value of $g = J_2/J_1$. The systems are here studied at their dimer-dilution percolation points $p^*$. The multi-critical point $(g^*, p^*)$ previously found for the bilayer is not reproduced for the single layer. Instead, there is line of critical points $(g < g^*, p^*)$ with continuously varying exponents. The uniform magnetic susceptibility diverges as $T^{-\alpha}$ with $\alpha \in [1/2, 1]$. This unusual behavior is attributed to an effective free-moment density $\sim T^{1-\alpha}$. The susceptibility of the bilayer is not divergent but exhibits remarkably robust quantum-critical scaling.

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which clearly is the same as for a single site-diluted layer, \( p^* \approx 0.41 \) (hole concentration) \[28\], there is a multii-critical point \((g^*, p^*)\) at which the long-range order on the percolating cluster vanishes and the spins are quantum-critical. A critical coupling \( g^* \approx 0.15 \) and dynamic exponent \( z^* \approx 1.3 \) were found in two independent QMC calculations \[15\] \[16\]. The generic transition for \( p < p^* \) has also been studied in detail by Monte Carlo simulations of an analogous 3D classical Heisenberg model with columnar defects \[17\]. Also here an exponent \( z \approx 1.3 \) was found (but \( z^* \neq z \) is expected because of the different cluster dimensionality). Long-range order in the presence of quantum fluctuations on the line \((g < g^*, p^*)\), which was believed not to be possible for a continuous order parameter \[30\], was recently related to the fracton dimensionality of the percolating cluster \[31\].

The question now arises as to the generality of the behavior found in the bilayer model. On its percolating cluster each spin has a neighbor in the opposite layer with which it correlates at low temperature. Magnetization fluctuations are thus quenched as \( T \to 0 \). Here the dimerized single-layer model is used to investigate the role of the bilayer symmetry upon dilution. Without disorder, the system has a quantum-phase transition, in the same universality class as the bilayer, at \( J_2/J_1 \approx 2.5 \). With dimer dilution again corresponding to random removal of \( J_2 \) dimers, the percolation point \( p^* = 1/2 \) because the dimers are connected as a triangular lattice \[28\]. The \( T = 0 \) phase diagram, outlined in Fig. 1 is similar to that of the bilayer in that there is a finite segment of the phase boundary at \( p = p^* \), terminating at a point \((g^*, p^*)\) beyond which the transition occurs for \( p < p^* \). However, as will be discussed in detail below, there is a striking difference: Whereas the percolating cluster of the bilayer has Néel order for \( 0 < g < g^* \) \[15\] \[16\], the percolating cluster of the single dimerized layer is quantum-critical on the whole line \((0 < g < g^*, p^*)\), with \( g^* \approx 1.25 \). On this line, the magnetization fluctuations are not completely quenched as \( T \to 0 \), leading to a divergent susceptibility, \( \chi \sim T^{-\alpha} \), with \( \alpha \to 1/2 \) for \( g \to g^* \) and \( \alpha \to 1 \) for \( g \to 0 \). For \( g = 0 \), a Curie susceptibility is expected on account of the percolating cluster breaking up into smaller pieces when all the \( J_2 \) couplings vanish (the percolation point here is \( p_0^* \approx 0.29 \)). Some of these clusters contain an odd number of spins. For \( g > 0 \), the divergent susceptibility can then be attributed to effectively isolated subclusters with net moments, which are gradually “frozen out” as the temperature is reduced. The form \( \chi \sim T^{-\alpha} \) corresponds to a free-moment density scaling as \( T^{1-\alpha} \). This remarkable behavior will here be demonstrated on the basis of large scale QMC (stochastic series expansion \[14\]) calculations. Only results exactly at the percolation threshold, \( p = p^* \), will be discussed. The numerical techniques and special methods developed for studies of random systems at ultra-low temperature are discussed in detail in \[20\].

The temperature dependence of the uniform susceptibility \( \chi(T) \) of the bilayer close to the multi-critical point was discussed before in Ref. \[15\] (averages over all clusters were presented in \[16\]). Fig. 2 shows a more extensive set of high-precision results for the largest cluster on \( L \times L \) lattices with \( L = 256 \) (\( L \to \infty \) converged for the temperatures shown) at \( p^* = 0.4072538 \[32\]. Averages over several thousand dilution realizations were taken. The temperature is scaled according to the expected quantum-critical form, \( \chi = a + bT^{d/z-1} \), where \( a \) and \( b \) are constants and \( a = 0 \) at a quantum-critical point. Using the fractal dimension \( d = 91/48 \) and adjusting \( z \) to obtain a linear \( \chi \) versus \( T^{d/z-1} \), the same dynamic exponent,
uniform susceptibility of the largest cluster was calculated for $L$ up to 256, down to $T = J/512 \ (L \to \infty$ converged). Here a special point ($g^*,p^*$) is found which separates qualitatively different behaviors of the uniform susceptibility. As seen in Fig. 3(a), at $g^* = 1.247 \pm 0.001$, $\chi$ is linear in $T$ and approaches a finite value as $T \to 0$. For $g > g^*$ the susceptibility drops to zero and for $g < g^*$ it diverges. As shown in Figs. 1(b), (c), the divergence is of the form $\chi \sim T^{-\alpha}$, with $\alpha$ very close to $1/2$ for $1 \lesssim g < g^*$ and $\alpha \to 1$ for $g \to 0$. Such a divergence can be interpreted as a temperature dependent fraction $\sim T^{1-\alpha}$ of effectively free magnetic moments.

As already noted, exactly at $g = 0$ the percolating cluster is broken up into smaller subclusters and then a Curie behavior, $\chi \sim T^{-1}$, is expected on account of clusters with a net spin. For small but non-zero $g$, one might then have expected a cross-over from Curie behavior when $T > g$ to a finite susceptibility as $T \to 0$. Instead, it appears that coupling the subclusters leads to a $g$ dependent power-law temperature scaling of the number of effectively free moments. The effective couplings of these moments to each other must thus have a $g$ dependent power-law distribution, leading to a self-similar structure of free moments different from that of the underlying fractal cluster. It is remarkable that this behavior persists also when $g \approx 1$, where the picture of weakly connected subclusters is not obviously relevant.

The bilayer percolating cluster is ordered at $T = 0$ for $g < g^*$ [15, 16]. This is not the case for the single dimerized layer at $p^*$. Instead, quantum-critical fluctuations are observed for $0 < g \leq g^*$. Consider the staggered structure factor $S(\pi, \pi)$ and susceptibility $\chi(\pi, \pi)$ of a cluster of $N_c$ spins,

$$S(\pi, \pi) = \frac{1}{N_c} \sum_{i,j} P_{ij} (S_i^1 S_j^2),$$

$$\chi(\pi, \pi) = \frac{1}{N_c} \sum_{i,j} P_{ij} \int_0^\beta d\tau \langle S_i^1(\tau) S_j^2(0) \rangle,$$

where $P_{ij} = (-1)^{z_i + y_i - z_j - y_j}$. At a quantum-critical point, these quantities, averaged over disorder, should scale with the system size as \langle $S(\pi, \pi)/N_c \sim L^{\gamma_s}$, $\chi(\pi, \pi)/N_c \sim L^{\gamma_\chi}$, with $\gamma_s = -(z + \eta)$ and $\gamma_\chi = -\eta$ (normalizing by $N_c \sim L^d$ before disorder-averaging leads to some reduction of statistical fluctuations). Fig. 4 shows results for $g = 1$. The observed scaling gives $z \approx 3.0$ and $\eta \approx -1.7$. The dynamic exponent can be compared with the expected quantum-critical susceptibility: $\chi \sim T^{-1-\alpha}$ with $\alpha = 1 - d/z$ [3]. With the exponent $\alpha = 1/2$ obtained from $\chi(T)$ in Fig. 3(b), it is apparent that this relationship does not hold here [z extracted from $S(\pi, \pi)$ and $\chi(\pi, \pi)$ should be the actual dynamic exponent]. At the special point $g^*$ the extracted $\alpha = 0$ and $z \approx d$ (not shown here) are in fact consistent with this relationship. This is also the case at the bilayer multicritical point [15]. The single-layer quantum-criticality

$z = 1.36 \pm 0.01$, is found for all $0 < g \lesssim g^*$. An improved estimate $g^* = 0.118 \pm 0.006$ is also obtained. Note that bilayer criticality can be expected only for $T < g$, which is indeed the case in Fig. 2.

In a clean quantum-critical system, there is a low-temperature cross-over of $\chi(T)$ to a "renormalized classical" behavior when $g < g_c$, at a temperature of the order of the spin stiffness $\rho_s$ [3]. No such cross-over is seen in Fig. 2 however. Although it cannot be completely excluded that there is a cross over at still lower temperature, one can also argue that there should be no cross-over, because $\rho_s = 0$ on the percolating cluster [15, 20] (although there is long-range order—this unusual behavior has also been discussed in [12]) and there is no apparent energy scale, except $T$, to govern the long-distance physics of the spins on this fractal network. Thus the multi-critical point $(p^*, g^*)$ may control the $T < g$ temperature dependence for all $0 \leq g \leq g^*$ at $p^*$. Considering the scaling in Fig. 2 extends down as low as to $T = J/256$ and to couplings $g \approx 1.247/3$, the results appear to support such an unusual manifestation of quantum-criticality on a fractal percolating cluster.

Turning now to the single-layer model at its dimer percolation point, $p^* = 1/2$ for $g > 0$, the disorder-averaged
on the line \((0 < g < g^*, p^*)\) thus appears to be fundamentally different. It should be noted that the behavior is not consistent with a Griffiths phase \([7]\), as the spin correlations in that case should be exponentially decaying, in contrast to the power-law seen in Fig. 3.

An extended line of quantum-critical points was not anticipated on the basis of a real space RG approach developed recently for quantum rotors on a percolating cluster \([31]\). The critical line discovered here for the single-layer model is more similar to the 1D random singlet phase \([5]\), in that there is a temperature dependent fraction of effectively free moments. In the random singlet phase \(z = \infty\) whereas in the model studied here \(z\) is finite and diverges in the limit \(g \to 0\). A temperature dependent fraction of effective moments has also been observed in a 2D model of interacting localized moments \([34]\). However, there the asymptotic \(T \to 0\) susceptibility is always Curie-like, and there is long-range order at \(T = 0\). An RG calculation for random frustrated moments in the continuum shows a \(\chi(T)\) divergence with varying exponent \([35]\). The ground state properties were not accessible in that study.

The bilayer multi-critical point \((p^*, g^*)\) has been argued \([15, 16]\) to influence finite-temperature properties of single-layer Zn doped cuprate antiferromagnets, for which a dynamic exponent \(z \approx 1.4\) was found in neutron scattering experiments \([21]\). However, although \(g^*\) is small \((\approx 0.12)\) it is difficult to explain how bilayer quantum-criticality could be realized when \(T > g = 0\) (due to an expected cross-over at \(T \approx g\); see Fig. 2). Physical realizations of single-layer dimer dilution are not immediately obvious. Nevertheless, the results presented here serve to illustrate rich and surprising behaviors arising from the interplay of classical percolation and quantum fluctuations, going beyond previous examples of scaling in percolating fractal structures \([36]\).

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