Low-energy dynamics of the two-dimensional S=1/2 Heisenberg antiferromagnet on percolating clusters

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We investigate the quantum dynamics of site diluted \( S = 1/2 \) Heisenberg antiferromagnetic clusters at the percolation threshold. We use Lanczos diagonalization to calculate the lowest excitation gap \( \Delta \) and, to reach larger sizes, study an upper bound for \( \Delta \) obtained from sum rules involving the staggered structure factor and susceptibility, which we evaluate by quantum Monte Carlo simulations. Scaling the gap distribution with the cluster length \( L \), we obtain a dynamic exponent \( z \approx 2D_f \), where \( D_f = 91/48 \) is the fractal dimensionality of the percolating cluster. This is in contrast to previous expectations of \( z = D_f \). We argue that the low-energy excitations are due to weakly coupled effective moments formed due to local imbalance in sublattice occupation.

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Antiferromagnets under doping with spinless vacancies exhibit interesting phenomena resulting from quantum fluctuations building on top of fluctuations of classical percolation. Various calculations for the two-dimensional (2D) Heisenberg model indicated that the quantum fluctuations for \( S = 1/2 \) are strong enough to cause a quantum phase transition at some vacancy concentration \( p = p_c \) less than the classical percolation threshold \( p^* \). However, recent quantum Monte Carlo (QMC) simulations have demonstrated that long-range order survives for all \( p \leq p^* \). Experiments on magnetically diluted layered cuprates agree with this, showing a low-temperature divergent correlation length up to the percolation point \( p_c \). The fractal percolating cluster at \( p^* \) is ordered. The dilution-driven phase transition is therefore a classical percolation transition of the static spin order, but quantum fluctuations present in the percolating cluster lead to changes in quantities related to the low-energy dynamics. The critical exponents depend on classical percolation exponents and the dynamic exponent \( z \) of the clusters, which thus becomes the focus of attention—it is the subject of this Letter.

The singlet-triplet gap of a clean \( D \)-dimensional antiferromagnet on a lattice of even length \( L \) scales as \( L^{-z} \) with \( z = D_f \). The lowest excitations are the quantum rotor states responsible for symmetry breaking when \( L \to \infty \). Vojta and Schmalian recently generalized this result to percolating clusters; \( z = D_f \), where in 2D the fractal dimensionality \( D_f = 91/48 \). QMC calculations by Yu et al. seem to confirm \( z = D_f \) at \( p^* \), however in an indirect way from the finite-temperature scaling \( \xi \sim T^{-1/2} \) of the correlation length. This form is expected for a quantum-critical system but is not necessarily related to the finite-size gap of ordered clusters. The exponent governing the finite-size gap is the one relevant to the \( T = 0 \) dilution transition. Here we will take a more direct approach, studying the scaling of the excitation gaps of percolating clusters. Our main result of this study is that the dynamic exponent is much larger than expected: \( z \approx 2D_f \). We will argue that the lowest excitations are due to weak interactions between moments formed by local sublattice asymmetry.

The diluted Heisenberg Hamiltonian is

\[
H = J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \mathbf{S}_i \cdot \mathbf{S}_j, \quad (J > 0),
\]

where \( \langle i,j \rangle \) are nearest neighbors on a 2D square lattice and \( \epsilon_i = 0, 1 \) with probability \( p \) and \( 1-p \). We focus on the percolation threshold, \( p = p^* \), and study the properties of clusters grown on an infinite lattice, keeping clusters of a target size \( N \) (see Ref. [3]). We first consider the gap \( \Delta = E_1 - E_0 \) between the singlet ground state and triplet first excited state of clusters with an equal number of spins in the two \((A,B)\) sublattices; \( N = n_A + n_B \), \( n_A = n_B \). We also discuss \( n_A \neq n_B \), for which the ground state is an \( S = |n_A - n_B|/2 \) multiplet, and find a subtle difference in the nature of the low-energy excitations.

Using Lanczos diagonalization, we study clusters with \( n \) up to 20. In order to reach larger sizes we use a QMC method (stochastic series expansion, SSE). Due to statistical errors, it is not possible to evaluate very small gaps directly using QMC. We therefore consider an upper bound \( \Delta^* \) for the gap,

\[
\Delta^* = 2S(\pi,\pi)/\chi(\pi,\pi) \geq \Delta,
\]

obtained from well known sum rules for the static structure factor \( S(q) \) and susceptibility \( \chi(q) \):

\[
\int_0^\infty \frac{d\omega}{\omega} S(q,\omega) = S(q),
\]

\[
2 \int_0^\infty \frac{d\omega}{\omega} \chi(q,\omega) = \chi(q),
\]

where \( S(q,\omega) \) is the dynamic structure factor. For a single mode \( \Delta^* = \Delta \). As in the undiluted system, we expect \( \Delta^* \) for Heisenberg clusters to scale as the true gap; \( \Delta^* \sim L^{-z/2D_f} \). At the very least, \( z \) obtained from \( \Delta^* \) will be a lower bound for the dynamic exponent.

In the SSE simulations we reach the ground state using a \( \beta = J/T \) doubling procedure, checking all clusters individually for \( T \to 0 \) saturation of \( \chi(\pi,\pi) \). Because of
the large \( z \), extremely low temperatures are required and we have therefore only gone up to \( n = 192 \), for which some clusters already require \( \beta = 217 \) \((S(\pi, \pi)\) saturates at significantly lower \( \beta \) \( [3] \)). The computational effort (CPU time and memory) scales as \( n^3 \) \( [12] \).

In Fig. 1 we show the probability distributions of the exact gap \( \Delta \) of clusters with \( n = 16, 18, \) and 20 obtained on the basis of \( 4 \times 10^4 \) samples for each size. We also show results for the upper bound \( \Delta^* \) for \( n = 16, 32, \) and 64 obtained from \( 6 \times 10^5 \) clusters each. A common feature for the small clusters is a double-peaked gap distribution. In the upper panel we show two illustrative clusters corresponding to the two peaks. Identifying pairs of spins likely to form singlets (giving a rough singlet-product approximation of the ground state) we find that the clusters of the lower peak always have “dangling spins” not belonging to a local singlet (for any reasonable pairing; the locations of the dangling spins are of course not unique), whereas dangling spins are absent for the upper peak. The large-gap peak vanishes as \( n \) grows; clearly because it is unlikely for a large cluster not to have any dangling spins. Dangling spins arise from local imbalance in sublattice occupation. They should act as weakly interacting moments, with effective couplings decreasing with separation. One should hence expect small gaps for clusters with dangling spins at large separation.

The role of isolated spins in the formation of long-range order has been pointed out by Bray-Ali and Moore \( [13] \). Although some spins can be very weakly coupled (effectively) to the rest of the cluster, correlations between them can be stronger than within the backbone of the cluster. Arbitrarily weakly coupled moments formed by groups of spins can also correlate over long distances and hence even a “sloppy” fractal cluster can order at \( T = 0 \) (a more thorough examination of long-range order was presented in \( [14] \)). Here we will argue that excitations involving localized effective moments are lower in energy than the quantum rotor states considered in previous discussions of the dynamic exponent \( \beta \).

Fig. 2 shows the size dependence of the disorder averages \( \langle \Delta \rangle \) and \( \langle \Delta^* \rangle \). A linear fit to \( \langle \Delta^* \rangle \) gives a slope \( z/D_f = 1.99(2) \), or \( z = 3.77(4) \). Although the small systems for which we have calculated the exact gaps are not yet in the scaling regime, the available \( \langle \Delta \rangle \) points reproduce well the shape of the \( \langle \Delta^* \rangle \) curve in the range where they overlap. Comparing the \( \Delta \) and \( \Delta^* \) distributions for \( n = 16 \) in Fig. 1 we also see that they are very similar—\( \Delta^* \) is only shifted up slightly relative to \( \Delta \).

The large \( z \) implies that the lowest excitations of these clusters are not quantum rotor states (which would give \( z = D_f \approx 1.89 \)). To investigate the nature of the excitations, we have calculated the local susceptibility:

\[
\chi_i = \int_0^\beta d\tau \langle S_i^z(\tau)S_i^z(0) \rangle,
\]

which can be used to define a local gap \( \Delta_i = 1/2\chi_i \), as in Eq. 2. The magnitude of the local gaps of three representative clusters are illustrated in Fig. 3. In the left cluster a few isolated sites with small gaps can be distinguished, whereas the small gaps are more spread out in the one to the right. In the central one there are isolated as well as more extended moments. Thus not only dangling spins but also other groups of spins can form effective moments. In all cases, the small-gap regions appear to be localized. Regions with large gaps can be seen where it is apparent that the connectivity favors local singlet formation. Such singlets can contribute to isolating the effective moments from each other.

Assuming that the low-energy physics of the clusters is governed by interactions between effective localized moments, we can apply concepts of the well-known strong-disorder renormalization group (RG) moment decimation.
procedure \(^{14,17,18}\) to analyze the low-energy behavior. The effective interactions between the moments can be ferromagnetic or antiferromagnetic, and we therefore have to consider two moments combining into either a smaller or a larger moment in each step \(^{10}\) (including the case of two equal moments forming a singlet and dropping out). On a cluster with \(n_A = n_B\) the decimation would ultimately leave two equal moments with an effective antiferromagnetic interaction. The lowest excitation is the singlet-triplet excitation of this pair. A key question is whether the typical size of the renormalized excitations due to finite local moment pairs.

The effective interactions between the moments can be described by extremal value statistics \(^{20,21}\) of the smallest local gaps, \(\Delta_{\min}\). We thus consider the distribution of \(\Delta_{\min}\) as a color coded mapping of \(-\ln(\Delta_i)\) to \([0,1]\) (for each cluster separately). The smallest gaps are \(\Delta_{\min} / J = 0.027\) (left), 0.014 (middle), and 0.012 (right). The largest gaps are \(\Delta_{\max} / J = 0.9\) (left and right) and 0.22 (middle).

If the excitations indeed are localized moment-pair excitations, the distribution of the first gap \((i.e., \Delta_i)\) should be described by extremal value statistics \(^{20,21}\) of the local gaps. We thus consider the distribution of \(\Delta_i\), taking into account a possible scaling with the system size, as suggested by the discussion above. We define \(\epsilon_i = \Delta_i / \Delta_i^{\Lambda^\omega} \sim \Delta_{\min}^{\Lambda^\omega} / D_i\). As shown in Eq. (7) for \(a \approx 2.8\) the distributions of \(\epsilon_i\) for different cluster sizes indeed collapse onto a single universal curve. For small \(\epsilon_i\), \(P(\epsilon_i) \sim A \epsilon_i^{-2}\), where \(\omega \approx 1\) and \(A\) is a constant. We want the distribution \(P_M(\epsilon_{\min})\) of the smallest local gap, \(\epsilon_{\min} = \Delta_{\min}L^\omega = \min\{\epsilon_1, \epsilon_2, \cdots, \epsilon_M\}\), for large \(M\). If the excitations are localized we have \(M \sim L^{D_f}\). Using the probability of a scaled local gap \(\epsilon' < \epsilon\),

\[
p(\epsilon') = \int_0^\epsilon P(\epsilon')d\epsilon' = \frac{A}{\omega + 1} \epsilon^{\omega + 1},
\]

we find the typical \(\epsilon_{\min}\) from \(p(\epsilon_{\min}) \sim M^{-1}\). Then using \(M \sim L^{D_f}\) we get \(\Delta_{\min} \sim L^{-a-D_f/\omega+1}\). Since \(\Delta_{\min}\) should scale as \(\Delta\) (which we have also confirmed numerically); \(\Delta_{\min} \sim L^{-z}\), we have

\[
z = a + \frac{D_f}{\omega + 1}.
\]

With \(a = 2.84\) and \(\omega = 1\) from the universal \(\Delta_iL^\omega\) curve in the upper panel of Fig. 4 we get \(z = 3.79\), in excellent agreement with the value 3.77(4) obtained in Fig. 4 on the basis of \(\Delta^*\). The full probability distribution of \(\Delta^*\) is also very consistent with \(\omega = 1\), as shown in the lower panel of Fig. 4. Here the best-fit dynamic exponent, \(z \approx 3.6\), is slightly smaller than the value quoted above, but considering the limited number of cluster sizes and samples the agreement is quite satisfactory. We conclude that the scaling behavior is consistent with low-energy excitations due to finite moment pairs.

We can also calculate the full distribution of \(\Delta\). Using \(P_M(\epsilon) = M P(\epsilon) [1 - p(\epsilon)]^{M-1}\), or

\[
P_M(\epsilon) = -\frac{d}{d\epsilon} [1 - p(\epsilon)]^M \simeq -\frac{d}{d\epsilon} e^{-M p(\epsilon)}
\]

and Eq. (6) gives the Frechet distribution \(^{20}\).

\[
P(u) = A u^a \exp(-A(\omega + 1)^{-1} u^{\omega + 1}), \quad u = u_0 \Delta L^z.
\]

This form can only be fitted to the \(\Delta^*\) data in Fig. 4 in the small-gap region. It is not completely clear to us why it fails for larger gaps, but there are signs of slower size-convergence on this side of the distribution. The deviations may also be related to the fact that we are studying the upper bound \(\Delta^*\), not the exact gap \(\Delta\).
For clusters with \( n_A \neq n_B \), the final result of the RG moment decimation procedure would not be two moments forming a singlet, but a single moment with spin \( S = |n_A - n_B|/2 \). The global sublattice imbalance would necessarily lead to moments that on average grow as the decimation proceeds, unlike in the case of \( n_A = n_B \) where it is possible that the effective moments reach a steady-state size as they are equally likely to grow or shrink at every RG step (a steady-state size is of course not guaranteed purely on statistical grounds, but our scaling study above supports it). The lowest excitation for an \( n_A \neq n_B \) cluster must hence involve spins scattered throughout the whole cluster. Considering that \( \langle S \rangle \sim \sqrt{n} \), such an excitation cannot be local. We indeed find that the exponent relation (7) is violated for clusters with even \( n \).

To conclude, we have presented a scaling study of the excitations of percolating \( S = 1/2 \) Heisenberg clusters, showing that the dynamic exponent \( z = 3.7(1) \); a factor 2 larger than \( z = D_f = 91/48 \) expected for quantum rotor states 5. We propose that the low-energy excitations are due to interactions between effective moments formed by local imbalance in sublattice occupation. We have used concepts of strong-disorder RG and extreme value statistics to derive a scaling relation, Eq. (7), between \( z \) and two exponents governing the scaling of local gaps, under the condition that the low-energy excitations involve a finite number of spins. For clusters with an equal number of spins on the two sublattices \( (n_A = n_B) \), this relation is satisfied by numerical results for an upper bound of the gap, \( \Delta^* \), defined in Eq. (2), and local gaps \( \Delta_i \) similarly defined. However, for clusters with \( n_A \neq n_B \) the global sublattice imbalance implies that the renormalized moments grow with system size. In accord with this non-locality we find that our exponent relation is violated. However, the dynamic exponent \( z \approx 2D_f \) for both \( n_A = n_B \) and \( n_A \neq n_B \) clusters.

Our scenario implies that once two identical clusters are coupled in a bilayer, with a small inter-layer coupling \( J_{\perp} \) (smaller than the value at which the long-range order vanishes 22), the low-energy excitations should change as effective moments in opposite layers completely compensate each other. Preliminary calculations for clusters with \( J_{\perp}/J \approx 0.05 \) indeed show a much smaller \( z \), consistent with \( z = D_f \) and the quantum rotor picture 3. This is also the case for the 3D classical Heisenberg model with columnar defects 24, which should describe the bilayer but not the single layer for which there are uncompensated Berry phases (local sublattice imbalance) not captured by the mapping to the classical model.

Another type of low-energy excitation possible in a percolating cluster is a fracton 24, 25. The fracton is localized for finite energy \( \Omega \), but delocalizes as \( \Omega \to 0 \). Hence, based on our scaling results for \( n_A = n_B \), it is different from our effective moment excitation. For a finite system \( \Omega(L) \propto L^{-D_{f}/d_f} \), where \( d_f \) is the fracton dimensionality. Approximate calculations of \( d_f \) 24 have given \( z_f = D_f/d_f \) smaller than the \( z \) reported here.

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