



Low-energy excitations of two-dimensional diluted Heisenberg quantum antiferromagnets

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We study the low-energy dynamics of $S=1/2$ antiferromagnetic Heisenberg clusters constructed by diluting a square lattice at vacancy concentration p at and below the percolation threshold $p^* \approx 0.407$. The finite-size scaling behavior of the average excitation gap, $\langle \Delta \rangle \sim L^{-z}$, where L is the cluster length, is obtained using quantum Monte Carlo results for an upper bound $\Delta^* > \Delta$, derived from sum rules. At the percolation threshold, we obtain a dynamic exponent $z = 3.6 \pm 0.1 \approx 2D_f$ for clusters with singlet ($S=0$) ground state. Here $D_f = 91/48$ is the fractal dimensionality of the percolating cluster. We argue that this large dynamic exponent—roughly twice that expected for quantum-rotor excitations—is a consequence of weakly interacting localized effective magnetic moments, which form due to local sublattice imbalance. This picture is supported by an extremal-value analysis of local spectral gaps, which delivers an exponent relation (between z and two exponents characterizing the local-gap distribution) reproduced by our simulation data. However, the average $\langle \Delta^* \rangle$ over all clusters, which have mostly ground-state spin $S > 0$, scales with a smaller exponent than for the $S=0$ clusters alone; $z \approx 1.5D_f$. Lanczos exact diagonalization for small clusters show that typically, $S \rightarrow S-1$ in the lowest-energy excitations while the dominant spectral weight originates from $S \rightarrow S+1$ excitations. Thus, the scaling of $\langle \Delta^* \rangle$ for clusters with ground state $S > 0$ does not reflect the lowest-energy excitations but the higher $S \rightarrow S+1$ excitations. This result can be understood within a valence bond picture. To further explore the scenario of localized moments, we introduce a classical dimer-monomer aggregation model to study the distribution of nearest-neighbor sites forming dimers (which are the objects used in mapping to the quantum-rotor model) and unpaired spins (monomers). The monomers are localized and, thus, effective magnetic moments should form in the spin system. We also study the lowest triplet excitation of $S=0$ clusters using quantum Monte Carlo calculations in the valence bond basis. The triplet is concentrated at some of the classical monomer regions, confirming the mechanism of moment formation. The number of spins (and moment regions) affected by the excitation scales as a nontrivial power of the cluster size. For a dimer-diluted bilayer Heisenberg model with weak interlayer coupling (where the system remains Néel ordered), there is no sublattice imbalance. In this case we find $z \approx D_f$, consistent with quantum-rotor excitations. For a single layer at $p < p^*$ we find $z \approx 2=D$, which indicates that the weakly interacting localized moment mechanism is valid only exactly at the percolation point. There is a crossover behavior close to the percolation point.

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I. INTRODUCTION

Two-dimensional (2D) antiferromagnets under doping with nonmagnetic impurities have emerged as interesting systems with rich possibilities to explore various disorder-driven phase transitions belonging to different universality classes.¹⁻⁶ Nonmagnetic impurities (vacancies) enhance quantum fluctuation by reducing the connectivity of the spins. Many earlier calculations⁷ for the 2D $S=1/2$ Heisenberg model had indicated that the quantum fluctuation can become strong enough to destroy the antiferromagnetic long-range order at a vacancy concentration p_c less than the classical percolation threshold p^* —whence p_c would be a quantum-critical point. However, more recent quantum Monte Carlo (QMC) simulations of the diluted quantum Heisenberg model,^{8,9} studies of effective classical systems,³ as well as experiments on $\text{La}_2\text{Cu}_{1-x}\text{Zn}_x\text{O}_4$ (with nonmagnetic Zn substituting $S=1/2$ Cu ions)¹⁰ all suggest that long-range order actually survives all the way up to the percolation point p^* , i.e., $p_c \equiv p^*$ for the single 2D layer.

The percolating cluster at p^* is ordered,⁹ which implies that the static properties at the dilution-driven transition in the quantum Heisenberg model scale as in the classical (percolation) problem. However, quantum fluctuations lead to

changes in the low-energy spin dynamics. The critical exponents therefore in general depend on classical percolation exponents as well as the dynamic exponent z of the quantum spin clusters.⁵ The dynamic exponent of the percolating cluster is therefore important and the focus of this paper.

The dynamic exponent governs the scaling of the gap Δ between the ground state and the lowest excited state of a finite cluster. With L denoting the cluster length (defined in some suitable way for a random cluster with irregular shape), the gap scales, on average, as $\langle \Delta \rangle \sim L^{-z}$. For a clean D -dimensional antiferromagnetic system on a bipartite lattice with N (even) sites, every spin can be paired up with a nearest-neighbor spin on the opposite sublattice to effectively form a “quantum rotor” with angular momentum $l = 0, 1$ states. In the mapping to a quantum-rotor model,¹¹ these local degrees of freedom are replaced with angular momenta l_i taking all integer values, with the high l_i states suppressed due to their energy being $\propto l_i^2$. The ground state of the coupled quantum-rotor system is a singlet. If the system is long-range ordered (but the global rotational symmetry has not been broken by any external perturbation), then the low-energy excitations of the coupled rotors (and the Néel ordered spin system¹²) are those of a single quantum rotor with mass $\propto N$. Thus $\Delta \sim N^{-1}$, i.e., $z=D$.

According to one recently proposed scenario for randomly diluted antiferromagnets,⁵ the quantum-rotor states remain the lowest-energy excitations even at p^* , where the dimensionality D_f of the percolating cluster is fractal; $z = D_f = 91/48$.¹³ Following the discussion above, this would seem to require that each spin can be paired up into a dimer with one of its nearest neighbors to effectively form a quantum rotor with $l=0$ ground state. This situation can be realized in the special case of the dimer-diluted bilayer¹ in which two coupled layers are diluted exactly in the same way by removing interlayer spin dimers. All the remaining spins can then be paired with spins on the opposite layer. At sufficiently weak interlayer coupling, the ground state of the largest connected cluster of spins in this system is long-range ordered for $p \leq p^*$ (Ref. 1) and, thus, the ground state should fall into the class of quantum-rotor states with gap $\propto N^{-1}$. However, in the case of a single diluted layer (or a bilayer with interlayer coupling $J_{\perp}=0$), there are in general some “dangling spins” (or more generally, regions with local sublattice imbalance) in which not all spins can be simultaneously paired up into nearest-neighbor dimers. One may still be able to pair spins over longer distances (which would also imply longer-range interactions between the rotors in the effective model) but at some point, when very long distances are required, the mapping to simple quantum rotors should break down.

Our assertion is that, at the percolation point, there are regions of spins that effectively form isolated magnetic moments, which cannot be described within an effective model containing only coupled rotors. The spatial distribution of these moment regions and weak effective interactions between them (mediated by the magnetically inert parts of the percolating cluster) lead low-energy excitations which are dramatically different from those of the quantum-rotor system. We introduced this scenario and presented supporting numerical evidence in a recent paper.¹⁴ Using finite-size scaling, we found a considerably larger dynamic exponent than the quantum-rotor value; $z \approx 2D_f$ instead of $z = D_f$. Here we provide more details of this work and also expand significantly on the previous calculations. We use several different methods to indirectly and directly examine the low-energy excitations of different types of clusters, both at and away from the percolation point.

The conclusion that $z \approx 2D_f$ for clusters at the percolation point is based largely on QMC calculations of an upper bound Δ^* to the lowest excitation gap Δ for finite clusters with singlet ($S=0$) ground states. The bound is defined using standard sum rules, discussed in detail in Sec. II B [and summarized as Eqs. (6), (9), and (10)]. The bound is exact, $\Delta^* = \Delta$, for a spectrum with a single mode and is known to scale with the system size in the same way as Δ more generally, e.g., in the clean Heisenberg model.²² It can be evaluated for large clusters using QMC calculations, in contrast to the exact gap, which is difficult to evaluate directly (because it is dominated by statistical errors if the gap is small). We also found that the probability distribution of local gaps Δ_i (also defined using a sum rule) scales with the system size.¹⁴ Defining $\epsilon_i = \Delta_i L^a$ (where the exponent is determined from simulation data and is $a \approx 2.8$ for $S=0$ clusters), the distribution $P(\epsilon_i)$ is size independent. Moreover, the low-energy tail

of this distribution is well described by a power law, $P(\epsilon_i) \propto \epsilon_i^{-\omega}$, with $\omega=1$. Analyzing the local gaps using extremal-value statistics, we found that the dynamic exponent should be related to the parameters of the local-gap distribution according to $z = a + D_f/(\omega + 1)$. Our simulation results satisfy this exponent relation remarkably well. The applicability of the exponent relation supports the notion that the low-energy excitations involve a number $\propto n$ finite regions (containing the effective moments) while an exponent $a > 0$ shows that individual excitations are not localized (since for localized excitations the energy should be independent of L for large L). The effective moments should be located in regions of imbalance in the number of spins on the two sublattices and many moments can be involved in an excitation. The value of the exponent a reflects the way in which the weak interactions between the effective moments involved in a particular excitation decrease with increasing system size, as these moments become further separated from each other.

In this paper, we report scaling results for larger clusters than previously and also compare results for clusters constructed in different ways. On the bipartite square lattice, we denote the number of sites on sublattices A and B as n_A and n_B , respectively. The ground state has spin $S = |n_A - n_B|/2$. We analyze in detail both $S=0$ and $S>0$ clusters at the percolation point p^* . We use the gap upper bound Δ^* from sum rules, as well as Lanczos exact diagonalization results for the excitation spectrum. For clusters with ground-state spin $S > 0$, we point out that the spectral weight entering in the sum-rule approach is dominated by $S \rightarrow S+1$ excitations, whereas the lowest-energy excitations typically correspond to $S \rightarrow S-1$. The quantity Δ^* in this case describes only excitations where $S \rightarrow S+1$, for which we find $z \approx 1.5D_f$ based on finite-size scaling. However, the lower $S \rightarrow S-1$ excitations most likely follow the same $z \approx 2D_f$ scaling as the $S=0 \rightarrow 1$ excitations of $n_A = n_B$ clusters. We also discuss results for the dimer-diluted bilayer at p^* , as well as the single layer at $p < p^*$. For these systems, we observe behavior consistent with quantum-rotor excitations (although other scenarios, e.g., fractons,^{15,16} are also possible).

To explain the existence of localized moments in the percolating cluster, we here also introduce a classical dimer-monomer aggregation model to study the purely geometrical local sublattice imbalance, which we believe is at the heart of this problem. The dimers correspond to nearest-neighbor sites that can form minimal local quantum rotors and the monomers lead to “dangling” spins that are, due to local sublattice imbalance, left over after the maximum number of dimers has formed. The monomers, individual ones or groups of several of them, can lead to effective magnetic moments in the spin system. We find that the classical monomers indeed are confined within regions of finite size, both at and away from the percolation point. The anomalous dynamics with $z \approx 2D_f$ in the single-layer quantum spin system at p^* should therefore be a consequence of localized quasifree magnetic moments interacting very weakly because of the vanishing spin stiffness of the percolating cluster.⁹ Away from the percolation point, the moments can lock to the global Néel order of the cluster (as a single magnetic impurity in two dimensional is known to do^{17,18}) and do not form an effective independent low-energy system.

To further investigate the nature of the excitations of the quantum spins and their relationship to the classical monomers, we have also applied a projector QMC method in the valence bond basis¹⁹ to directly study the triplet excitations of clusters with singlet ground states. In the valence bond basis, a triplet state can be described by a lone triplet bond, the location of which fluctuates among the background singlet bonds. We find that the triplet bond is indeed predominantly localized at a subset of the classical monomer regions. The total size of the excitation (i.e., the number of spins involved in it) is not finite, however, but grows with the cluster size according to a nontrivial power law.

The outline of the rest of the paper is as follows. After defining the spin models and describing several computational methods in Sec. II, we present results of both Lanczos exact diagonalization and sum-rule QMC calculations for single-layer clusters at $p=p^*$ in Sec. III. In Sec. IV we discuss the distribution of spectral weight in the dynamic structure factor originating from excited states of different total spin, using Lanczos exact diagonalization as well as an approximate analysis based on valence bond states. We discuss scaling results for percolating bilayer clusters in Sec. V and for single-layer clusters away from the percolation point in Sec. VI. The classical dimer-monomer aggregation model is discussed in Sec. VII and results of the valence bond projector QMC simulations of triplet excitations in Sec. VIII. We conclude in Sec. IX with a summary and discussion.

II. MODEL AND METHODS

The Heisenberg Hamiltonian on a single-site-diluted layer is given by

$$H = J \sum_{\langle i,j \rangle} \delta_i \delta_j \mathbf{S}_i \cdot \mathbf{S}_j, \quad (J > 0), \quad (1)$$

where $\langle i,j \rangle$ denotes nearest neighbors on a 2D square lattice and $\delta_i=0$ (vacancy) and $\delta_i=1$ (magnetic site) with probability p and $1-p$, respectively. We study clusters with two types of boundary conditions. In open-boundary $L \times L$ systems, we start with all magnetic sites and introduce vacancies with probability p . We study the largest cluster of connected magnetic sites. The number of spins n in such clusters fluctuates and scales as $\langle n \rangle \sim L^{D_f}$, with $D_f=91/48$. We also study clusters grown on an infinite lattice. Starting from a single magnetic site, we add more sites to the cluster with probability $1-p$ by transversing along the boundary sites, leaving sites unfilled with probability p but flagging each site as visited (so that sites assigned as vacancies are not visited again). This procedure terminates at random at some stage where all neighbors of the cluster have been assigned as vacancies. We only keep clusters of some desired target size n . These clusters have a characteristic average length $\langle L \rangle$ (defined, e.g., as their radius of gyration) such that $n \propto \langle L \rangle^{D_f}$. The two types of clusters will be referred to as $L \times L$ and fixed n , respectively. In Ref. 14, we only studied fixed- n clusters. Here we also consider the $L \times L$ variant to check whether the finite-size scaling properties depend on the boundary conditions in the cluster construction. For $p < p^*$, we consider only the $L \times L$ clusters because the fixed- n construction rarely terminates at reasonably small n in this case.

Under each type of boundary condition, we further consider two different ensembles of sublattice occupations; $n_A = n_B$ in which case all clusters have ground-state spin $S=0$, as well as arbitrary $n = n_A + n_B$ (with the distribution give by the cluster construction), corresponding to ground-state spin $S = |n_A - n_B|/2$. The latter ensemble includes also the $S=0$ clusters.

A bilayer cluster is constructed by coupling two identical single-layer clusters with an interlayer coupling constant J_\perp . The Hamiltonian is thus

$$H = J \sum_{\langle i,j \rangle} \delta_i \delta_j (\mathbf{S}_{1i} \cdot \mathbf{S}_{1j} + \mathbf{S}_{2i} \cdot \mathbf{S}_{2j}) + J_\perp \sum_i \delta_i \mathbf{S}_{1i} \cdot \mathbf{S}_{2i}, \quad (2)$$

where the subscripts 1 and 2 refer to the two layers. Also in this case we can study $L \times L$ or fixed- n clusters but, in contrast to the single layer, the ground state of a bilayer cluster is always a singlet because each spin can be paired with its neighbor in the opposite layer. We consider small coupling ratios J_\perp / J , for which the ground state has long-range order.¹

Here our main interest is in the energy gap Δ between the ground state and the first excited state, which in the case of an $n_A = n_B$ cluster is a singlet-triplet gap. For clusters with general n_A, n_B such that $S = |n_A - n_B|/2 > 0$, the lowest excitation can have total spin $S' = S - 1, S$, or $S + 1$. In addition to the gap, the distribution of the spin S' of the lowest-energy excitation is also interesting. We will also study the localization properties of the excitations very explicitly, by formulating the problem in the valence bond basis and carrying out unbiased quantum Monte Carlo calculations of $S' = 1$ excitations of clusters with $S=0$ ground states.

To calculate the gaps, we use both direct and indirect (approximate, through sum rules) estimates, using the methods discussed in Secs. II A and II B. In Sec. II C we will introduce the valence bond QMC scheme for directly imaging the spatial distribution of triplet excitations.

A. Exact diagonalization

The most straight-forward approach is to diagonalize the Hamiltonian numerically in sectors of different magnetization,

$$m_z = \sum_{i=1}^n S_i^z, \quad (3)$$

using the Lanczos method. However, for irregular clusters (without lattice symmetries to exploit for block diagonalization), this can be done in practice only for up to $n \approx 20$ spins, due to the rapid growth of the matrix sizes with n (considering also that we have to average over a large number—typically thousands—of random-cluster realizations). Nevertheless, such calculations are very useful and give some important insights into the role of dangling spins in low-energy excitations.

In addition to studying the level spectrum, focusing on a few low-lying states and calculating their total spin to classify the excitations, we also compute the full dynamic spin structure factor (in the standard way with the Lanczos method, as described, e.g., in Ref. 20),

$$S(\mathbf{q}, \omega) = \sum_m |\langle m | S_{\mathbf{q}}^z | 0 \rangle|^2 \delta(\omega + E_0 - E_m), \quad (4)$$

where $S_{\mathbf{q}}^z$ is the Fourier transform of the spin operators,

$$S_{\mathbf{q}}^z = \frac{1}{\sqrt{n}} \sum_{j=1}^n e^{i\mathbf{q}\cdot\mathbf{r}_j} S_j^z. \quad (5)$$

In a clean Heisenberg antiferromagnet on a bipartite lattice, the lowest excitation is a triplet at $q=(\pi, \pi)$. We can use this wave vector also for the diluted system, although the momentum is no longer conserved, i.e., the energy eigenstates $|m\rangle$ in Eq. (4) are not classified by the quantum number \mathbf{q} but the spin operators $S_{\mathbf{q}}^z$ are still completely well defined. We expect $S(\pi, \pi, \omega)$ to exhibit the largest spectral weight for the low-energy excitations since these should involve out-of-phase fluctuations of neighboring spins. As we will see in Sec. III C, the dynamic structure factor is of great utility in judging the validity of our sum-rule-based approach for an upper bound of the energy gap, which we discuss next.

B. Quantum Monte Carlo and sum rules

We use the stochastic series-expansion (SSE) QMC method²¹ to calculate quantities which are closely related to the gap. An upper bound Δ^* to the ground-state energy gap Δ can be obtained using the static spin structure factor $S(\mathbf{q})$ and susceptibility $\chi(\mathbf{q})$ at the staggered wave vector $\mathbf{q}=(\pi, \pi)$,

$$\Delta^* = 2S(\pi, \pi)/\chi(\pi, \pi) \geq \Delta. \quad (6)$$

For a cluster of n sites the static staggered structure factor is computed according to

$$S(\pi, \pi) = \frac{1}{n} \left\langle \left(\sum_{i=1}^n (-1)^{\phi_i} S_i^z \right)^2 \right\rangle \quad (7)$$

and the corresponding susceptibility as

$$\chi(\pi, \pi) = \frac{1}{n} \left\langle \sum_{i,j=1}^n (-1)^{\phi_j - \phi_i} \int_0^\beta d\tau S_i^z(\tau) S_j^z(0) \right\rangle, \quad (8)$$

where $\phi_i = x_i + y_i$ gives the staggered phase, with x_i and y_i the (integer) site coordinates.

The upper bound to the gap [Eq. (6)] follows from the well-known sum rules,

$$\int_0^\infty d\omega S(\mathbf{q}, \omega) = S(\mathbf{q}), \quad (9)$$

$$2 \int_0^\infty \frac{d\omega}{\omega} S(\mathbf{q}, \omega) = \chi(\mathbf{q}), \quad (10)$$

which, in the way written here, are valid at temperature $T=0$ for any wave vector \mathbf{q} . In a system with a sole triplet mode (a hypothetical situation) with energy $\omega_{\mathbf{q}}$, we get $2S(\mathbf{q})/\chi(\mathbf{q}) = \omega_{\mathbf{q}}$. Any spectral weight above this lowest mode will render the ratio larger than $\omega_{\mathbf{q}}$. For a clean system, the lowest quantum-rotor state is at $\mathbf{q}=(\pi, \pi)$ (whereas at other wave vectors spin waves are the lowest excitations). As

we discussed above, we expect $\mathbf{q}=(\pi, \pi)$ to be the best choice for examining low-energy excitations also in the diluted system and we here focus exclusively on this case.

The staggered structure factor and susceptibility can be efficiently calculated with the SSE method with “operator-loop” updates.²¹ Disorder averages are subsequently calculated for the ratio in Eq. (6) (where, it should be stressed, we first evaluate the ratio separately for each cluster in order to obtain the gap bound specifically for each of them and then take the average) using, typically, thousands of random realizations of either the largest cluster on $L \times L$ lattices or fixed- n clusters.

For a clean Heisenberg antiferromagnet, Δ^* is known²² to scale with the system size as the true gap; $\langle \Delta^* \rangle \sim \langle \Delta \rangle \sim L^{-z}$. This is because the dominant spectral weight is at the very lowest excitation energy—the spectral function in the thermodynamic limit has a delta function at the lowest energy, followed by a continuum at higher energies. We expect similar spectral features in the percolating cluster and suspect that Δ^* should scale as Δ (and will show supporting numerical results in the next section). At the very least, if the true power-law behavior is $\langle \Delta \rangle \sim L^{-z} \sim n^{-z/D_f}$, then the value \tilde{z} extracted from finite-size scaling of Δ^* must be a lower bound to the true dynamic exponent. Actually, in Sec. III we will use Lanczos results for the dynamic structure factor on small clusters to show that the finite-size scaling of Δ^* does not reflect the true lowest-energy excitations in the case of $S>0$ clusters but all indications are that the sum-rule approach is valid for $S=0$ clusters.

We will also study an effective local (site-dependent) excitation gap

$$\Delta_i = \frac{1}{2} \frac{1}{\chi_i}, \quad (11)$$

which is analogous to the gap bound [Eq. (6)] but here the “local structure factor” is just a constant; $S_i = (S_i^z)^2 = 1/4$. The local susceptibility χ_i is defined as

$$\chi_i = \int_0^\beta d\tau \langle S_i^z(\tau) S_i^z(0) \rangle. \quad (12)$$

Although the imaginary-time-dependent correlation function $\langle S_i^z(\tau) S_i^z(0) \rangle$ is asymptotically, for $\tau \rightarrow \infty$, dominated by the lowest excitation, in practice the integral will be dominated by the excitation(s) which predominantly affects the given site i . For a disordered system, different sites can be affected by different excitations and Δ_i then represents a typical energy scale of excitations affecting spin i .

We should note that for clusters with ground-state spin $S>0$, the grand-canonical SSE method samples over all magnetization sectors $-S \leq m_z \leq S$.²¹ We therefore have to subtract the static ($\omega=0$) contributions in Eqs. (7), (8), and (12) arising from a nonzero m_z , i.e., in Eq. (12) we subtract $\beta \langle S_i^z \rangle^2$ computed in the different m_z sectors and averaged over all m_z .

The SSE method operates at $T>0$ but we can achieve the $T \rightarrow 0$ limit by choosing T sufficiently low for all quantities of interest to converge. We use a “ β doubling” procedure⁹ in which the inverse temperature is successively doubled until

there is no longer any detectable dependence of calculated quantities on β . Since the dynamic exponent is large, the temperature $T \ll \Delta$ has to be very low indeed for large clusters. As an example of the ultralow temperatures required, the largest β we use for $n=512$ clusters with $S=0$ is $\beta = 2^{19} \approx 5 \times 10^5$. Since the simulation (CPU) time and memory usage scale essentially linearly in both β and n , these calculations are quite demanding. Fortunately, the SSE code for the isotropic Heisenberg model can be effectively parallelized²³ and we have run most of the simulations on a massively parallel computer very well suited for these calculations.²⁴

When studying disorder averaged static properties, the SSE runs for each individual cluster can be rather short. As long as each run is properly equilibrated (for which the β -doubling procedure also helps⁹), the average over many realizations will give an unbiased estimate to any simple average, e.g., a spin correlation function. However, when computing nonlinear functions involving several quantities, such as the ratio [Eq. (6)], the statistical errors introduce a bias. It is therefore important to collect sufficient statistics for the individual clusters. We have compared results of runs of different lengths in order to make sure that the results presented here do not suffer from significant bias effects.

C. Valence bond projector Monte Carlo

To study the nature of the lowest triplet excitation of clusters with $S=0$ ground states, we apply a valence bond projector Monte Carlo method.^{19,25} This method has been described in detail in recent papers^{26,29} and we here only review the elements necessary to understand the way we can access the triplet excitations and study their spatial distribution on the clusters.

First, consider the singlet ground state $|0\rangle_s$, which we want to project out from a singlet “trial” state $|\Psi\rangle_s$. The latter has an expansion in all singlet energy eigenstates,

$$|\Psi\rangle_s = \sum_n c_n |n\rangle_s. \quad (13)$$

In the standard way, if the ground-state energy is the eigenvalue of the Hamiltonian which is the largest in magnitude, which can always be assured by subtracting a constant from H (which we assume has been done, if necessary), the ground state can be projected out by applying a high power of H to the trial state,

$$(-H)^P |\Psi\rangle = c_0 (-E_0)^P \left[|0\rangle_s + \frac{c_1}{c_0} \left(\frac{E_1}{E_0} \right)^P |1\rangle_s + \dots \right], \quad (14)$$

where we include the minus sign because normally $E_0 < 0$. For large P all the excited states are filtered out because the ratios $|E_n/E_0| < 1$.

Valence bond basis states are products of $N/2$ singlets,

$$(i,j) = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j) / \sqrt{2}, \quad (15)$$

where we consider the first, i , and second, j , spins to always be on sublattices A and B , respectively. The trial state is thus expressed in this overcomplete basis as

$$|\Psi\rangle_s = \sum_v w_v |(i_1^v, j_1^v), \dots, (i_{N/2}^v, j_{N/2}^v)\rangle = \sum_v w_v |V_v\rangle, \quad (16)$$

where v labels all the different tilings of the cluster into valence bonds, of which there are $(N/2)!$ different ones, and we have introduced the short-hand notation $|V_v\rangle$ for a valence bond basis state.

For a trial state in a ground-state projector calculation, it is convenient to use an amplitude product state,^{27,28} where the expansion coefficients are given by

$$w_v = \prod_{x,y} h(x,y)^{n_v(x,y)}, \quad (17)$$

where $h(x,y) > 0$ and $n_v(x,y)$ is the number of bonds of size (x,y) in the configuration, i.e., the length of the bond is $r = (x^2 + y^2)^{1/2}$. Note that it is not necessary to normalize the trial state (which would anyway be difficult to do).

For the clean 2D system, the optimal amplitudes are translationally invariant and decay as $h(r) \sim r^{-3}$.²⁸ For random clusters, the optimal amplitudes are naturally not translationally invariant. While the average bond probabilities (which are related to the amplitudes) decay with r , for any given cluster there are typically some regions spanned by long bonds (a feature intimately connected with the low-energy physics, as we will discuss in Secs. IV and VIII). One could in principle optimize all the $\propto n^2$ different amplitudes for each specific cluster. However, the effort involved in individual optimizations for hundreds or thousands of clusters does not necessarily pay off, compared to just projecting the trial state with a somewhat larger power P of H . We here use a very simple trial state with all $h(x,y) = 1$.

To carry out the projection using Monte Carlo sampling, we write the $S=1/2$ Heisenberg Hamiltonian in terms of singlet projection operators on all the pairs b of nearest-neighbor sites $\langle i(b), j(b) \rangle$,

$$H_b \equiv H_{i(b),j(b)} = - \left(\mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)} - \frac{1}{4} \right) \quad (18)$$

and write the projection operator in Eq. (15) as

$$(-H)^P = \left(\sum_{b=1}^{N_b} H_b \right)^P = \sum_r \mathcal{P}_r, \quad (19)$$

where

$$\mathcal{P}_r = H_{b_m^r} \cdots H_{b_2^r} H_{b_1^r} \quad (20)$$

denotes the possible strings, $r=1, \dots, N_b^P$, of the singlet projectors.

When a singlet projector H_{ij} acts on a state with a valence bond on the two sites i, j , the state remains unchanged with a matrix element of unity; we call this a diagonal projection. If the operator acts on a state with no valence bond on the two sites, then the two bonds (i, k) and (l, j) connected to i, j are broken, and new singlets (i, j) and (l, k) are formed. This process has matrix element $1/2$ and we call it an off-diagonal projection. Thus the projection rules are

$$H_{ij} |\cdots (i, j) \cdots\rangle = |\cdots (i, j) \cdots\rangle, \quad (21)$$

$$H_{ij}|\cdots(i,k)\cdots(l,j)\cdots\rangle = \frac{1}{2}|\cdots(i,j)\cdots(l,k)\cdots\rangle. \quad (22)$$

Acting on a component $|V_a\rangle$ of the trial state, a string \mathcal{P}_r effects a number of rearrangements [Eq. (22)] of pairs of valence bonds, resulting in another valence bond basis state which we call $|V_a(r)\rangle$,

$$\mathcal{P}_r|V_a\rangle = W_{ar}|V_a(r)\rangle. \quad (23)$$

Here the ‘‘projection weight’’ W_{ar} for a combination of operator string \mathcal{P}_r and state $|V_a\rangle$ is given by the number $m_{\text{off}}(a,r)$ of off-diagonal operations [Eq. (22)] in the course of the projection,

$$W_{ar} = 2^{-m_{\text{off}}(a,r)}. \quad (24)$$

The expectation value of an operator A can be written

$$\begin{aligned} \langle A \rangle &= \frac{\sum_{ab} \sum_{rl} w_a w_b \langle V_b | \mathcal{P}_l^* A \mathcal{P}_r | V_a \rangle}{\sum_{ab} \sum_{rl} w_a w_b \langle V_b | \mathcal{P}_l^* \mathcal{P}_r | V_a \rangle} \\ &= \frac{\sum_{ab} \sum_{rl} w_a w_b W_{ar} W_{bl} \langle V_b(l) | A | V_a(r) \rangle}{\sum_{ab} \sum_{rl} w_a w_b W_{ar} W_{bl} \langle V_b(l) | V_a(r) \rangle}. \end{aligned} \quad (25)$$

where w_a and w_b are the weights computed according to Eq. (17) for the bonds in the states $|V_a\rangle$ and $\langle V_b|$ in the expansion [Eq. (16)] of the trial ket $|\Psi\rangle_s$ and bra $\langle\Psi|_s$ states.

The sampling weight to be used in Monte Carlo calculations of Eq. (25) is

$$W(a,b,r,l) = w_a w_b W_{ar} W_{bl} \langle V_b(l) | V_a(r) \rangle, \quad (26)$$

where the overlap of the two projected states is given by

$$\langle V_b(l) | V_a(r) \rangle = 2^{N_0 - N/2}, \quad (27)$$

where N_0 is the number of loops formed when the bond configurations of the states $|V_a(r)\rangle$ and $\langle V_b(l)|$ are superimposed (forming the transposition graph²⁷). Simple sampling procedures for the operator strings and trial state bonds are described in Refs. 19 and 26. More efficient sampling methods have been developed recently,²⁹ which we use but do not discuss here.

For the purpose of the present paper, the most interesting aspect of the valence bond projector scheme is the fact that we can easily extend the scheme to also study a triplet state. A trial wave function in the triplet sector can be expressed in the overcomplete basis of a lone triplet bond among $N/2 - 1$ singlets. We denote a zero-magnetization triplet by square brackets,

$$[i,j] = (\uparrow_i \downarrow_j + \downarrow_i \uparrow_j) / \sqrt{2} \quad (28)$$

and expand the triplet trial state as

$$\begin{aligned} |\Psi\rangle_t &= \sum_v w_v \sum_{m=1}^{N/2} |(i_1^v, j_1^v) \cdots [i_m^v, j_m^v] \cdots (i_{N/2}^v, j_{N/2}^v)\rangle \\ &= \sum_v w_v \sum_{m=1}^{N/2} |V_{v,m}\rangle, \end{aligned} \quad (29)$$

where the normalization is again irrelevant. Here we use the same expansion coefficients—the amplitude products [Eq. (17)]—as in the singlet trial state. Note that for a clean system, the singlet state [Eq. (16)] has momentum $\mathbf{k}=(0,0)$, whereas the triplet [Eq. (29)] has $\mathbf{k}=(\pi,\pi)$. These are the known momenta of the lowest states in the two spin sectors (with the triplet being the lowest member of Anderson’s tower of quantum-rotor states¹²). The wave-function signs corresponding to Eqs. (16) and (29) should be correct for the lowest singlet and triplet states also for a diluted system since all conditions for Marshall’s sign rule [which corresponds to all positive expansion coefficients in Eq. (29)] (Ref. 30) remain valid.

When acting on a triplet bond, the singlet projector H_{ij} destroys the state while the action between a singlet bond and a triplet bond is very similar to the pure singlet rules [Eq. (22)]. The two triplet rules are

$$H_{ij}|\cdots[i,j]\cdots\rangle = 0, \quad (30)$$

$$H_{ij}|\cdots[i,k]\cdots(l,j)\cdots\rangle = \frac{1}{2}|\cdots(i,j)\cdots[l,k]\cdots\rangle. \quad (31)$$

In the projector method, it is straight forward to convert one bond of the singlet trial wave function into a triplet and trace its evolution. The triplet states that survive after all P operations [i.e., that are not destroyed by a diagonal operation, Eq. (30)] are used to measure properties in the triplet sector. To measure triplet expectation values, we have to project triplets like this both in the bra and ket in the triplet version of Eq. (25). We also have to check the overlap [Eq. (26)] of the surviving triplet states. One can show that the two triplet bonds have to be in the same transposition-graph loop in order for the overlap to be nonzero and it is then equal to the singlet overlap [Eq. (27)]. For surviving pairs of triplets, the weight of the triplet configuration is the same as that of the original singlet one. One can therefore sample the configurations in the singlet sector and carry out measurements with all the surviving triplets *without reweighting*. This is one of the strengths of the valence bond projector method.

There can still be problems with this approach because the number of surviving triplets decreases with the projection power P [because the probability of a triplet to be destroyed by a diagonal triplet operation, Eq. (30), increases]. It helps considerably that the starting trial state can have the triplet at $N/2$ different locations, in both the bra and the ket states, and as long as one pair out of the total of $(N/2)^2$ combinations survives (and gives nonzero overlap), we can collect statistics. One can carry out the summation over triplet locations m in Eq. (29) efficiently, without introducing any additional factor $N/2$ in the computational effort, in a single traversal of the operator sequence.

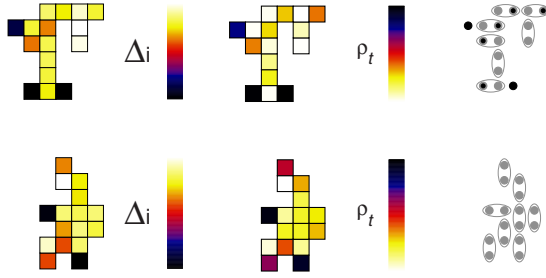


FIG. 1. (Color online) Results for two different clusters, visualized with color scales, of the QMC sum-rule approximation of local gaps Δ_i (left) and valence bond projection calculation of the triplet density ρ_t (center). To the right, the clusters are shown covered with dimers (pairs of spins enclosed by ovals) and left-over monomers (black circles). The black circles inside ovals indicate other possible locations of the monomers, corresponding to alternative maximal dimer coverings (which here always corresponds to two left-over monomers).

In some cases it can still happen that the triplet quantities of interest have not converged well to the $P \rightarrow \infty$ limit before the triplet survival probability becomes too low to be useful. This is not a serious problem in the present application, although an extrapolation to infinite P based on several calculations with reasonable triplet survival probability is necessary to ensure that the results represent the lowest triplet. An exponential asymptotic convergence can be expected based on Eq. (15). We will discuss the convergence with P in more detail in Sec. VIII, where Fig. 17 shows examples for relatively large clusters, for which P on the order of 10^3 – 10^4 times the cluster size n is required to reliably extract the properties of the lowest triplet.

We will discuss the spatial distribution of the triplets. The surviving triplet states have the triplet bond located at two particular sites (which can be different in the ket and the bra, and we do the measurements in both of these states). In a random system, the average triplet density will not be uniform and provides a very concrete measure of the localization properties of the lowest triplet excitation.

Note that the distribution of the $m_z=0$ triplet bond is equivalent to the magnetization distribution in a state with $m_z=1$, which could also be studied using the SSE method at low temperatures (e.g., by including a weak magnetic field³¹). However, the valence bond states also contain other relevant information, e.g., the statistics of the length of the triplet bond, which can only be accessed in the valence bond basis and which will be useful for analyzing the nature of the excitations (as we will do in Sec. VIII).

D. Examples

Having introduced the technical aspects of all the methods, we now present illustrative results for two small clusters. This will help to clarify the subsequent analysis and discussion of results for larger clusters.

The local gaps Δ_i and the triplet density ρ_t are visualized for two different clusters in Fig. 1. Here the color scales were created separately for the two clusters, with the minimum

and maximum values for each quantity on a particular cluster corresponding to the extrema of the scales shown (and, thus, the plots should only be used to examine the variations within the clusters, not comparing the values for the two clusters).

The two clusters differ qualitatively in a way which is directly related to our arguments pertaining to a low-energy scale. The lower cluster can be completely subdivided into pairs of nearest-neighbor sites (dimers, represented by ovals), whereas the upper one has two dangling spins left (monomers, shown as black circles outside ovals) after the sites have been paired up as much as possible. The pairing into dimers is not unique—the black circles inside ovals show all other possible monomer locations for this cluster. In all cases there are two monomers in two separate regions. The classical dimer-monomer aggregation model discussed in Sec. VII contains the statistics of the distribution of the monomers. Our main argument is that the presence of monomer sites leads to small gaps, i.e., a large dynamic exponent. For the two clusters shown, the exact gaps are $0.039J$ and $0.276J$, respectively, for the cluster with and without monomer sites. The gap upper bounds Δ^* are $0.076J$ and $0.35J$. While, in particular, the former is quite far from the exact result (in a relative measure), the difference between the two clusters is still large.

Large clusters are likely to have dangling spins and the top cluster in Fig. 1 is therefore the more interesting case. One can clearly see a strong correspondence between small local gaps and large triplet density, and they both coincide very well with sites where monomers can be located. Although this is in accord with the notion of monomers leading to finite regions of spins affected by the excitation, these clusters are clearly too small to give any meaningful quantitative insights into the localization properties of the triplet. In the following four sections we will carry out quantitative scaling analyses of the gaps in different types of clusters while further discussion of the monomer and triplet distributions will be postponed to Secs. VII and VIII, respectively.

III. SINGLE-LAYER GAP SCALING AT THE PERCOLATION POINT

We here discuss the distribution of exact gaps obtained with the Lanczos method, as well as SSE QMC results for the gap upper bound and local gaps. First we consider $S=0$ clusters ($n_A=n_B$) and then arbitrary S .

A. Clusters with singlet ground state

Figure 2(a) shows the probability distribution of the logarithm of the exact gap Δ of $n=16$ clusters obtained using 4×10^4 samples. We also show results for the upper bound Δ^* for clusters of the same size, obtained from SSE calculations for 6×10^3 different clusters. We presented these results in Ref. 14 and here regraph them in a different way for added clarity. The Δ^* curve is visibly shifted up in energy relative to the Δ distribution (with the average $\Delta^*/\Delta \approx 1.5$) but the

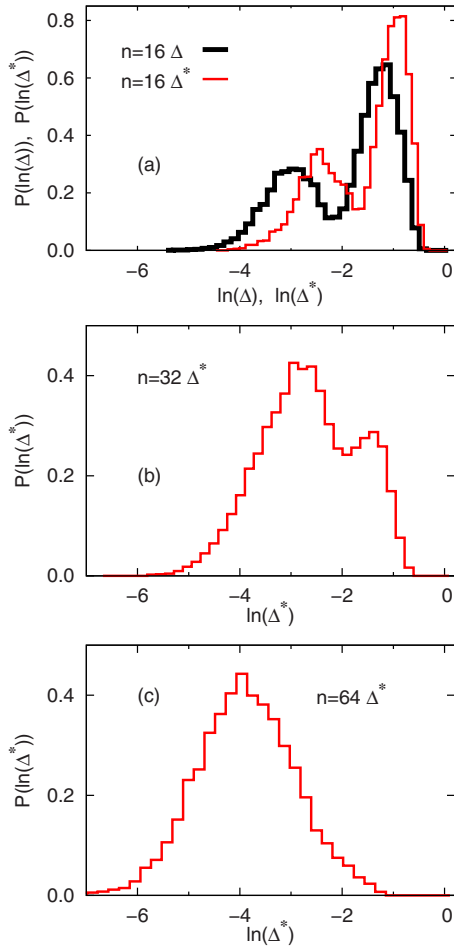


FIG. 2. (Color online) Distribution of the singlet-triplet gap Δ and its upper bound QMC estimate Δ^* for (a) $n=16$ clusters, and the Δ^* distribution for (b) $n=32$ and (c) $n=64$.

shapes of the two curves are remarkably similar. The two-peak structure is related to the dangling spins discussed in Sec. II D. The large-gap peak originates almost exclusively from clusters that can be completely partitioned into nearest-neighbor dimers, whereas the low-gap peak corresponds to clusters with dangling spins (monomers). Clearly, as the cluster size grows, it will be less and less likely to find clusters with no monomers and the weight of the high-energy peak should therefore gradually diminish and be absent for large clusters. The relative size of the large- Δ^* peak is indeed much smaller in the $n=32$ distribution graphed in Fig. 2(b). In the $L=64$ histogram, shown in panel (c), only a single peak can be discerned (with only a weak tail suggesting some remaining contributions from no monomer clusters).

Figure 3 shows the size dependence of the disorder averaged $\langle \Delta^* \rangle$ on log-log scales for both fixed- n (top panel) and $L \times L$ (bottom panel) clusters. We also show the typical values $\langle \Delta^* \rangle_t$, obtained by averaging $\ln(\Delta^*)$ for the individual clusters. While the typical and average values do not exactly coincide, for large systems they scale in the same way. Linear fits to the $\langle \Delta^* \rangle_t$ data on the log-log scales gives $z = 3.6 \pm 0.1$ for both types of clusters. Here the estimated error reflects the purely statistical errors of the line fits in combination with small variations depending on what range of system sizes are included.

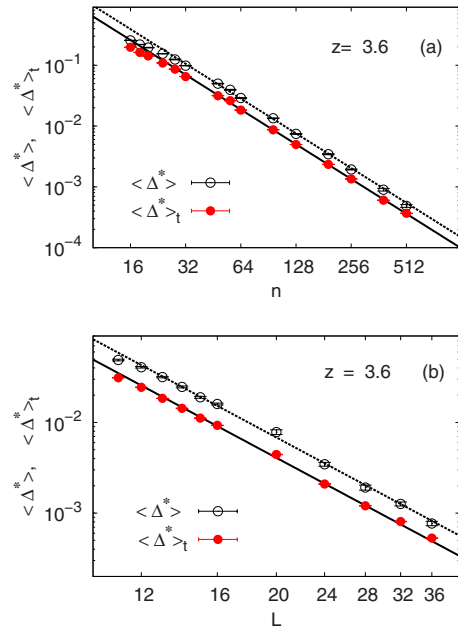


FIG. 3. (Color online) Finite-size scaling of the average $\langle \Delta^* \rangle$ and typical $\langle \Delta^* \rangle_t$ gap upper bound for $S=0$ ($n_A=n_B$) clusters. The top and bottom panels show results for fixed- n and $L \times L$ clusters, respectively. The lines correspond to the scaling expected with dynamic exponent $z=3.6$ (i.e., the size dependence is $\sim n^{-z/D_f}$ and $\sim L^{-z}$, respectively, for the two types of clusters).

As shown in Figs. 4(a) and 5(a), for fixed- n and $L \times L$ clusters, respectively, not only do the averages and typical values of Δ^* scale with the system size but the entire distribution can be collapsed onto a common size-independent

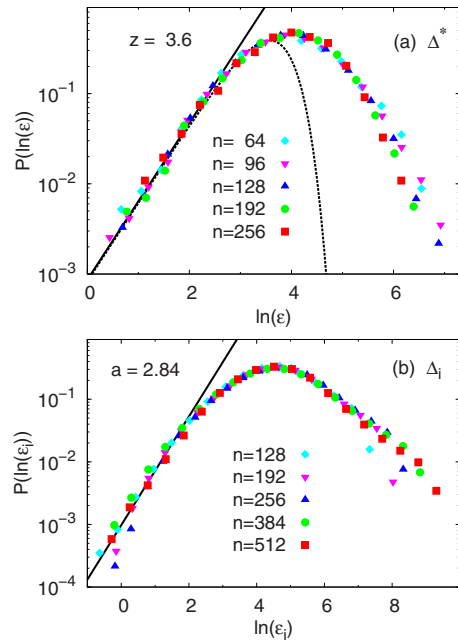


FIG. 4. (Color online) Distribution of the logarithm of the (a) scaled gap upper bound $\epsilon = \Delta^* n^{z/D_f}$ and (b) local-gap bound $\epsilon_i = \Delta_i n^{a/D_f}$ for fixed- n clusters with ground-state spin $S=0$. The exponents are indicated in the panels. The solid lines correspond to small-gap exponent $\omega=1$ and the curve in (a) is a Fréchet form.

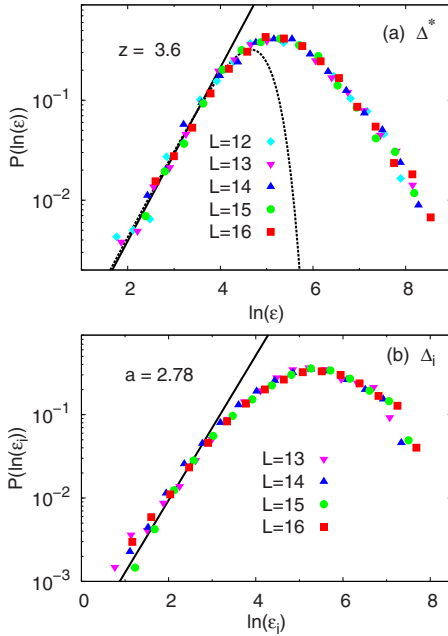


FIG. 5. (Color online) Probability distribution of the logarithm of the (a) scaled gap upper bound $\epsilon = \Delta^* L^z$ and (b) local-gap bound $\epsilon_i = \Delta_i L^a$ for $L \times L$ clusters with ground-state spin $S=0$. The solid lines correspond to $\omega=1$ and the curve in (a) is a Fréchet form.

curve, by scaling the gap estimates with the cluster size. We define the scaled gap upper bounds for the two types of clusters according to

$$\epsilon = \begin{cases} \Delta^* L^z, & (L \times L \text{ clusters}), \\ \Delta^* n^{z/D_f}, & (\text{fixed-}n \text{ clusters}). \end{cases} \quad (32)$$

As can be seen in the figures, the small-gap side of the distribution of $\ln(\epsilon)$ is very well described by a power law; $P[\ln(\epsilon)] \propto \epsilon^{\omega+1}$, with $\omega=1$. This distribution of the logarithm of ϵ corresponds to a probability distribution $P(\epsilon) \sim \epsilon^{-\omega}$ for the scaled gap ϵ itself [since the differential $d \ln(\epsilon) = d\epsilon/\epsilon$].

We next consider the local gap estimate Δ_i , i.e., the inverse local susceptibility [Eq. (12)]. Measuring this quantity at each site, we define size-scaled local gaps,

$$\epsilon_i = \begin{cases} \Delta_i L^a, & (L \times L \text{ clusters}), \\ \Delta_i n^{a/D_f}, & (\text{fixed-}n \text{ clusters}). \end{cases} \quad (33)$$

The probability distributions of $\ln(\epsilon_i)$ for different cluster sizes, based on several hundred clusters of each size, collapse onto each other for a suitably chosen $a \approx 2.8$, as shown in Figs. 4(b) and 5(b) for the two types of clusters. The small-gap tails of the distributions are again very well described by a power law; $P(\epsilon_i) \sim \epsilon_i^{-\omega}$, with the same $\omega=1$ as for the scaled “global” gap bound Δ^* .

It should be noted in Figs. 4 and 5, and in several figures to follow, that we do not show any statistical error bars for the individual data points. The statistics (number of counts) at the low and high ends of the distribution is relatively poor, which is reflected in some scatter of the data (consistent with the statistics) around the fitted power laws at the low end.

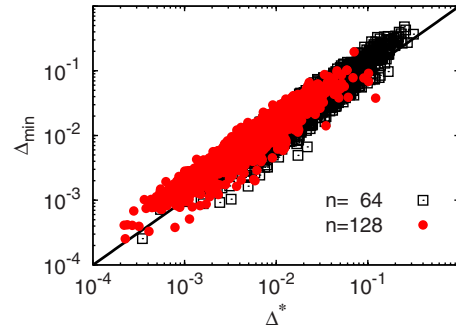


FIG. 6. (Color online) Correlations between the smallest local gap Δ_{\min} and the gap upper bound Δ^* for clusters of size $n=64$ and 128 . Each data point corresponds to Monte Carlo results for a randomly generated $n_A=n_B$ cluster. The line shows the ideal (single-mode) case of complete equivalence of the two estimates of the finite-size gap.

B. Extremal-value analysis

In Ref. 14 we used extremal-value statistics³² (in a way generalizing a treatment of localized excitations by Lin *et al.*³³) and found a relationship between the exponents z , a , and ω . For completeness, we repeat and further clarify our arguments here.

Our hypothesis is that, for a large cluster of size n , there is a number $\propto n$ of regions of sublattice imbalance. These regions act as localized magnetic moments, which interact weakly with each other through the magnetically inert parts of the percolating cluster. The excitations of this effective low-energy system of coupled moments are not localized because several distant moments can be involved. It is then natural to expect some size dependence of the local gaps, due to the dependence of the effective interactions on the distance between the moments involved in a low-energy excitation, combined with the increasing distance (on average) between these moments with increasing cluster size. We posit that this size dependence can be captured by the single exponent a in Eq. (33).

The actual finite-size gap Δ for a given cluster should correspond to the smallest of the local gaps Δ_i for that cluster, for which we use the notation Δ_{\min} . Of course, the local gaps that we measure are only approximations; one cannot unambiguously define a local gap in an interacting system. Nevertheless, Δ_i reflects the local distribution of spectral weight and there should be some site i within the regions affected by the lowest excitation for which $\Delta_i = \Delta_{\min} \approx \Delta$ (and $\Delta_{\min} \geq \Delta$). In our numerical analysis, Δ is approximated by the bound Δ^* and we expect $\Delta_{\min} \approx \Delta^*$. Examining the numerical data, we indeed find a very strong correlation between the two quantities, as shown in Fig. 6 for fixed- n clusters. Here it can be seen that Δ_{\min} is typically 1.5–2 times larger than Δ^* , which reflects larger spectral weight above the true lowest excitation energy in the local dynamic structure factor $S_i(\omega)$ than in $S(\pi, \pi, \omega)$. It should be noted that $\Delta_{\min} < \Delta^*$ is allowed within the sum-rule approach, although $\Delta_{\min} \geq \Delta$ has to hold strictly.

We now assume that there is a number $M \propto n$ of different local scaled gaps ϵ_i and investigate the consequences of this

in light of the scaling behavior found above. We assume a probability distribution $P(\epsilon_i) = A\epsilon_i^\omega$ for some window of small ϵ (where A is a constant and we consider a more general case than just $\omega=1$ extracted from the finite-size scaling of the data). We derive the probability distribution for the smallest scaled local gap $P_M(\epsilon_{\min})$ for large $M \sim L^{D_f}$ using extremal-value statistics.

We should clarify why we assume $M \propto n$ for the number of local gaps, instead of just $M=n$, which is the actual number of different numerical values Δ_i that we compute for a given cluster. The distinction will not matter in the analysis but it has an important physical significance. In our scenario, a cluster consists of regions with localized moments, which participate in the low-energy excitations, as well as inert parts which have only high-energy excitations. The form of the probability distribution $P(\epsilon_i) = A\epsilon_i^\omega$ should only hold for sites i within the moment regions. It is then important in our analysis that also the number of such sites scales as n (although one could also generalize to $M \sim n^\gamma$ with $\gamma < 1$ but the consistency of our analysis with $M \propto n$ will show that this is not necessary). Later, we will provide more concrete proof that the moment regions are finite and the total number of spins belonging to moments grows linearly with n .

Note also that in reality the distribution of local gaps must be cut off (equals zero exactly) below some very small value for a given finite cluster size. However, this should not affect the results of the analysis to follow because also the assumed power-law probability is very small below such a threshold. We thus expect the results derived below to be valid within some significant window of scaled gaps ϵ .

We denote the probability of finding a local gap at an arbitrary chosen site (within one of the moment regions) smaller than some value x by $P_{<}(x)$. It is given by

$$P_{<}(x) = \int_0^x P(\epsilon_i) d\epsilon_i = \frac{A}{\omega+1} x^{\omega+1}. \quad (34)$$

If one of the scaled gaps ϵ_j is the smallest and has the value ϵ , then all the other ($M-1$ different) values ϵ_i , $i \neq j$ must be larger than ϵ . The probability of these $M-1$ values being smaller than ϵ is $[1 - P_{<}(\epsilon)]^{M-1}$. Since any of the M values could be the smallest one, we get a factor of M and finally the distribution of the ϵ_j value is given by $P(\epsilon_j)$. Thus, the distribution of the smallest scaled local gap is

$$P_M(\epsilon) = MP(\epsilon)[1 - P_{<}(\epsilon)]^{M-1}, \quad (35)$$

which for small ϵ also can be expressed as

$$P_M(\epsilon) = -\frac{d}{d\epsilon}[1 - P_{<}(\epsilon)]^M \simeq -\frac{d}{d\epsilon}e^{-MP_{<}(\epsilon)}. \quad (36)$$

Using Eq. (34) here gives the Frechet distribution,³²

$$P_F(u) = Au^\omega \exp[-A(\omega+1)^{-1}u^{\omega+1}], \quad (37)$$

where $u = u_0\epsilon$. Thus, the probability distribution of the scaled global gap should be governed by the same exponent ω as the scaled local gaps. The Frechet form can indeed be fitted to the Δ^* data in Figs. 4(a) and 5(a), with the same exponent $\omega=1$ as in the local-gap (b) panels but only in the small-gap region. One cannot expect the Frechet distribution to work

for large gaps since the local-gap distribution we started from is linear only in the small ϵ_i region (and, as discussed above, we expect the large-gap part of the distribution to be dominated by excitations of the magnetically inert cluster regions without moments). The fitted forms in Figs. 4(a) and 5(a) are therefore also not normalized. Nevertheless, it is encouraging that the data is in agreement with the result that both the local and global gaps should scale with the same exponent, which here is $\omega=1$.

Let us now use the distribution [Eq. (34)] in a different way. Since we assume that there are $M \propto n$ local gaps, the typical smallest gap should correspond to $P_{<}(x)$ for which $x = M^{-1}$, i.e., $x \propto L^{-D_f}$. This gives $\Delta_{\min} \propto L^{-a-D_f(\omega+1)}$. Since Δ_{\min} should equal Δ and, by definition, $\Delta \propto L^{-z}$, we arrive at the following relationship between the three exponents:

$$z = a + \frac{D_f}{\omega+1}. \quad (38)$$

This generalizes the relation $z = D_f/(\omega+1)$ used as a criterion for a localized excitation by Lin *et al.*³³ to excitations originating from two or more finite entangled regions distributed over the cluster. With our numerical values from the finite-size scaling above, $z \approx 3.6$ and $\omega=1$ (the latter of which is not based on a fit but is a value consistent with all our results), we obtain $a \approx 2.65$, in very reasonable agreement with the value $a \approx 2.8$ obtained in Figs. 4(b) and 5(b) from the scaling of the ϵ_i data for the fixed- n and $L \times L$ clusters. The applicability of the exponent relation [Eq. (38)] provides strong support to our hypothesis of ‘‘globally entangled local-moment excitations.’’

C. SSE results for general- S clusters

We now turn to clusters with no restriction on the sublattice occupations n_A and n_B in the generated ensemble. Scaling results for the global and local gaps of $L \times L$ clusters are shown in Fig. 7. The finite-size scaling of the average and typical values of Δ^* are shown for both fixed- n and $L \times L$ clusters in Fig. 8. We obtain $a \approx 2.1$ and $z \approx 2.8$ for both cluster types. These exponents differ significantly from the ones obtained previously for the ensemble including $S=0$ clusters only. In particular, $z \approx 1.5D_f$, whereas the $S=0$ clusters gave $z \approx 2D_f$. The exponent relationship [Eq. (38)] still holds approximately, albeit with somewhat larger deviations than in the $S=0$ case. The small-gap behavior remains consistent with the exponent $\omega=1$ in all cases.

We believe that the much smaller exponents z, a are due to a failure of the sum-rule approach to capture the true low-energy states for $S > 0$. To demonstrate this, we next investigate the dynamic structure factor [Eq. (4)].

IV. SPECTRAL WEIGHT DISTRIBUTION

We will investigate how the spectral weight of the dynamic structure factor is distributed among different spin sectors of the excited states in Eq. (4). Acting on the ground state with the $\mathbf{q} = (\pi, \pi)$ spin operator [Eq. (5)], or the corresponding x or y components, on one of the $(2S+1)$ degenerate ground states of spin S results in states with spin S and

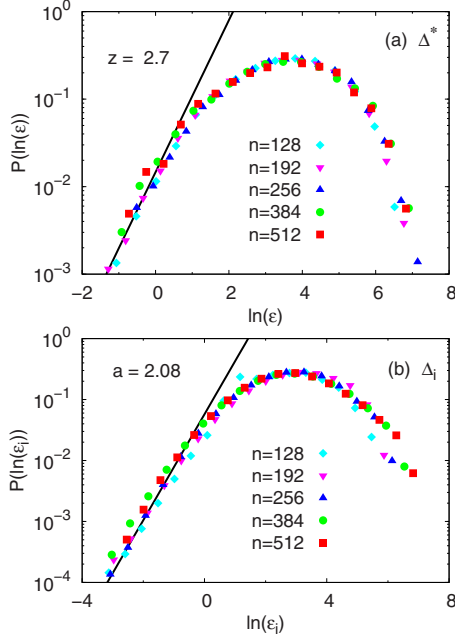


FIG. 7. (Color online) Distribution of the (a) scaled gap upper bound and (b) local gaps of $L \times L$ clusters with no restriction on the sublattice occupation numbers n_A and n_B . The solid line shows the asymptotic small-gap behavior expected with $\omega=1$.

$S \pm 1$. This well-known selection rule for the dynamic structure factor [Eq. (4)] can be easily demonstrated in the valence bond basis. Here we do this as a prelude to discussing the distribution of the spectral weight among the three sectors of final spin for clusters with ground state $S > 0$.

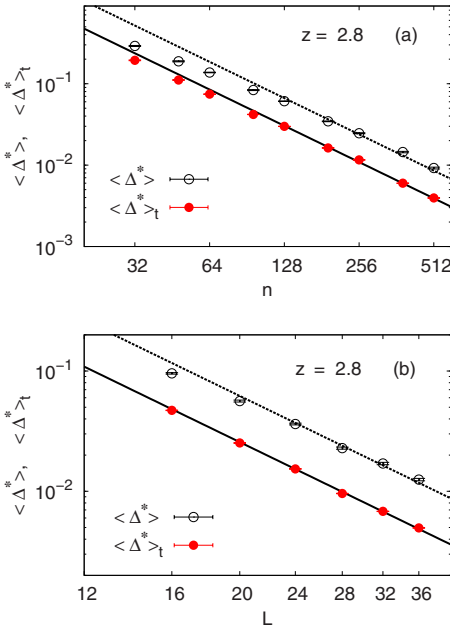


FIG. 8. (Color online) Finite-size scaling of the average and typical gap upper bound Δ^* for the ensemble with unrestricted n_A and n_B . The upper and lower panels show results for fixed- n and $L \times L$ clusters, respectively. Lines corresponding to a dynamic exponent $z=2.8$ are shown with all the data sets.

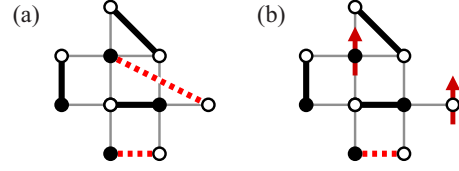


FIG. 9. (Color online) Valence bond states on a cluster with sublattice imbalance $\Delta_{AB}=1$ (requiring one nonbipartite bond—here the top one). Open and solid circles indicate the two sublattices. Singlet and triplet bonds are shown as solid and dashed lines, respectively. (a) shows a state with two triplet bonds and $m_z=0$. In (b), there are two unpaired up spins and $m_z=1$.

A. Selection rules

We consider an extended valence bond basis with an arbitrary number of $m_z=0$ triplet bonds [Eq. (29)] in addition to singlet bonds, for a state with total $m_z=0$ (hence the number of spins, N , is even). Later, we will consider also $m_z \neq 0$. The standard valence bond basis for $n_A=n_B$ is restricted to bipartite bonds only.²⁷ Here, for $n_A \neq n_B$ and $m_z=0$, we require a maximal number of bipartite bonds, i.e., if the total sublattice imbalance is defined as $\Delta_{AB}=|n_A-n_B|/2$, there will be $n_b=N/2-\Delta_{AB}$ bipartite bonds and $n_c=\Delta_{AB}$ bonds connecting sites on the same sublattice (with all such pairs either on the A or B sublattice, depending on which sublattice has the larger number of sites). This basis is clearly overcomplete. A state with two triplet bonds and one nonbipartite bond is illustrated in Fig. 9(a).

First, let us discuss the relationship between the total spin S and the number of triplet bonds. A state with n_t triplets does not have fixed spin when $n_t > 1$ (while for $n_t=0$ and 1 , the state has fixed $S=0$ and 1 , respectively). According to the rules for addition of angular momenta, one might at first sight suspect that n_t triplets could be used to form states with $S=0, 1, \dots, n_t$. However, consider the operator Z which inverts all the spins,

$$Z|S_1^z, S_2^z, \dots, S_N^z\rangle = |-S_1^z, -S_2^z, \dots, -S_N^z\rangle, \quad (39)$$

which is a special case of a rotation in spin space. Since the total magnetization $m_z=0$, a state with fixed S is also an eigenstate of this operator, with eigenvalue $z = \pm 1$. Since a triplet pair (bond) is even under Z while a singlet pair is odd, the eigenvalue z of a state with a fixed number n_t of triplet bonds is $z = (-1)^{N/2-n_t}$. Thus, in order to construct a state with fixed S (fixed z), one cannot mix valence bond states with even and odd number of triplets. Since the minimum number of triplets required to construct a state with fixed spin is $n_t = S$, we conclude that the triplet numbers that can be mixed are $n_t \in \{S, S+2, \dots, N/2\}$. This, in turn, implies that a state with fixed number of triplets is a linear combination of states with $S \in \{0/1, \dots, n_t-2, n_t\}$, where the lower limit 0 or 1 applies for even and odd S , respectively.

Next, we let the $q=(\pi, \pi)$ spin operator [Eq. (5)] act on a given valence bond state with n_t triplets. We can write the operator in a way tailored specifically for the state under consideration,

$$S_{\pi,\pi}^z = \frac{1}{\sqrt{N}} \left[\sum_{b=1}^{n_b} (S_{i(b)}^z - S_{j(b)}^z) + \sum_{c=1}^{n_c} (S_{k(c)}^z + S_{l(c)}^z) \right]. \quad (40)$$

Here the subscripts $i(b)$ and $j(b)$ refer to two sites connected by a bipartite valence bond b and $k(c), l(c)$ denotes a pair of sites on the same sublattice, connected by a nonbipartite bond c . The bonds can be singlets or triplets and the possible outcomes when operating with one of the terms are

$$\begin{aligned} (S_{i(b)}^z - S_{j(b)}^z) |\cdots(i_b, j_b)\cdots\rangle &= |\cdots[i_b, j_b]\cdots\rangle, \\ (S_{i(b)}^z - S_{j(b)}^z) |\cdots[i_b, j_b]\cdots\rangle &= |\cdots(i_b, j_b)\cdots\rangle, \\ (S_{i(c)}^z + S_{j(c)}^z) |\cdots(i_c, j_c)\cdots\rangle &= 0, \\ (S_{i(c)}^z + S_{j(c)}^z) |\cdots[i_c, j_c]\cdots\rangle &= 0. \end{aligned} \quad (41)$$

Thus, operating with the full $S_{\pi,\pi}^z$ we obtain a linear combination of states with n_t+1 and n_t-1 triplets. Extending this result to the case of a fixed- S state $|\Psi_S\rangle$, which is a linear combination of states with different n_t (all even or all odd), we can think of the triplet bond created or destroyed in each term [with the operator, Eq. (40), written in the appropriate way for operation on each term] as adding or subtracting a spin 1 to or from a spin S . Then, considering also that even and odd S corresponds to mixtures of even and odd n_t , respectively, we conclude that the state $S_{\pi,\pi}^z |\Psi_S\rangle$ is a mixture of only $S \pm 1$ states (which is also consistent with the fact that for $S=0$ ground states, the spectral weight is exclusively due to $S=1$ excitations).

In order to respect the spin-rotational invariance when using the z -component operator $S_{\pi,\pi}^z$ in the dynamic structure factor for $S>0$, we also have to consider nonzero m_z . Some of the spins are then not paired up into valence bonds. In a minimal basis mixing valence bonds and spins, there are $2m_z$ unpaired up or down spins for $m_z>0$ and $m_z<0$, respectively. The unpaired spins cannot be restricted to the same sublattice, so now the basis consists of the unpaired spins at arbitrary locations, a maximal number of bipartite bonds on the remaining locations, and the rest of the sites covered by nonbipartite bonds. An example of such a state is illustrated in Fig. 9(a).

In Eq. (40) n_b and n_c are the number of bipartite and nonbipartite bonds in a given basis state and $n_b+n_c=n-m_z$. We now also have to add a sum over the $2m_z$ unpaired spins. It is then clear that $S_{\pi,\pi}^z |\Psi_S\rangle$ will contain also a spin- S component, arising from this added sum, in addition to the $S \pm 1$ components (which can be argued for in analogy with the $m_z=0$ case). Some, but not all, of the corresponding spectral weight in the spin S sector is at $\omega=0$, as discussed in Sec. II B. Averaging over all $m_z=-S, \dots, S-1, S$, it is also clear that the amount of $S \rightarrow S$ spectral weight should increase with S , as it is zero for $S=0$ and the relative weight of the operations on unpaired spins increases with m_z .

B. Results for small clusters

We now turn to numerical results for the dynamic structure factor. Investigating small clusters with the Lanczos

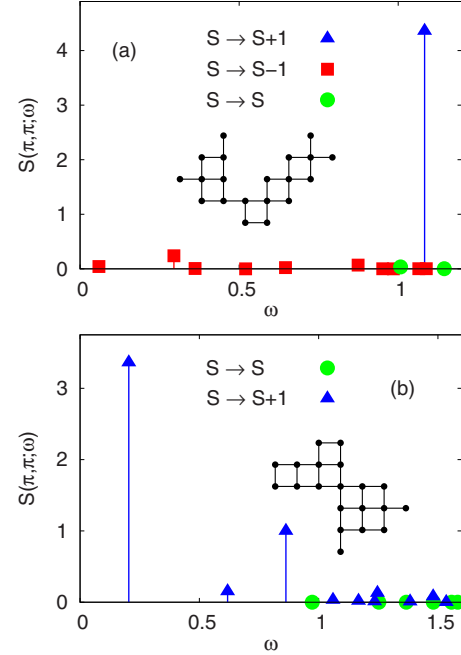


FIG. 10. (Color online) Dynamic structure factors of two 20-site clusters with ground-state spin (a) $S=3$ and (b) $S=0$. The cluster shapes are drawn in the panels. The delta functions in Eq. (4) are represented by vertical lines of length equaling the spectral weight. The symbols on top of the line indicate the spin of the corresponding excited states relative to the ground state S . In (b), there is no $S \rightarrow S$ spectral weight; the circles only indicate the locations of such states.

method, we have found that the lowest excitation of a cluster with ground-state spin S almost always has spin $S-1$, whereas the dominant spectral weight arises from a state with $S+1$. An example of this behavior is shown in Fig. 10(a) for a cluster with ground-state spin $S=3$. The spectrum is dominated by a large contribution from an $S=4$ state at $\omega/J \approx 1$. However, there are numerous very small contributions from $S=2$ states below this peak, including the lowest excitation at $\omega/J \approx 0.05$. In this case the sum rules give a bound Δ^* very close to the energy of the lowest $S=4$ state and, thus, differs from the true gap Δ by a factor of 20. In contrast, Fig. 10(b) shows results for a cluster with $S=0$ ground state. Here there are of course no excitations with $S-1$ and all the spectral weight is in the $S+1=1$ channel. Moreover, the dominant weight originates from the lowest excitation. The sum-rule approach here gives a bound reasonably close to the true gap.

We further examine the statistics of the gaps corresponding to excitations with $S \pm 1$ for $n=20$ clusters with ground state S . In Fig. 11 we show histograms based on several hundred clusters with $S=1, 2, 3$, along with results for $S=0$ clusters for comparison. We can see that the distribution of the $S+1$ excitations is peaked at higher energies than the $S-1$ ones and the distance between the two distributions grows with S . As we discussed in Sec. III A, the distribution of singlet-triplet excitation gaps is double-peaked for small systems, with the upper peak diminishing as a function of the cluster size. In Fig. 11 the lower part of the $S=0 \rightarrow 1$

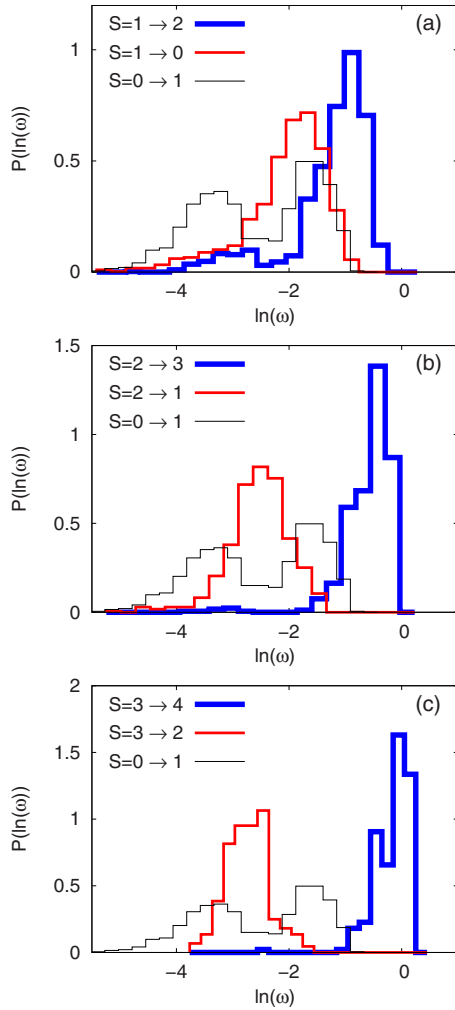


FIG. 11. (Color online) Distribution of the energies of the lowest excitation with $S=S \pm 1$ in $n=20$ clusters with ground-state spin S . Results for $S=1,2,3$ are shown in panels (a)–(c). In all panels, results for the lowest triplet excitation of $S=0$ clusters are shown for comparison.

distribution is located below the $S-1$ distributions for $S > 0$ clusters. It appears plausible from these results that the $S \rightarrow S-1$ and $S \rightarrow S+1$ gaps can have different scaling properties.

It is clear from these calculations that the sum-rule approach for $S > 0$ clusters does not reflect the true smallest gaps, which are due to $S-1$ excitations but instead reflect the distribution of spectral weight of $S+1$ excitations. The quantity Δ^* therefore has a different meaning, which can still be physically relevant because many experimental techniques probe $S(q, \omega)$ directly, e.g., neutron scattering and nuclear magnetic resonance. These experiments should observe low-energy dynamics corresponding to $z \approx 1.5D_f$ according to our results in the previous section. The most plausible scenario is that the lowest $S-1$ excitation energies, for large clusters and typical ground-state spin (which is of the order \sqrt{n}), scale with the same dynamic exponent $z \approx 2D_f$ as the triplet excitations of $S=0$ clusters (which we will argue further also in the next section). While their low spectral weights would make them difficult to observe in measure-

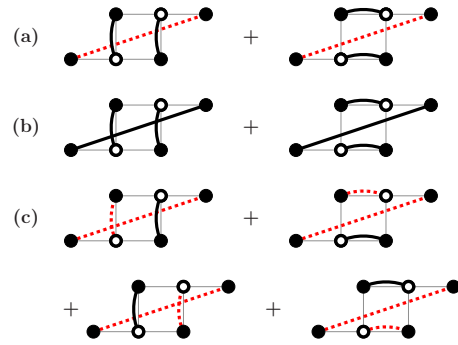


FIG. 12. (Color online) Valence bond states corresponding closely to true eigenstates of a six-site cluster with ground-state spin $S=1$. Solid and dashed bonds correspond to singlets and triplets, respectively. (a) is the ground state, (b) the lowest $S=0$ excitation, and (c) is obtained from (a) by acting on it with $S^z_{\pi, \pi}$ (which is a good approximation to the lowest $S=2$ excitation).

ments sensitive to $S(q, \omega)$, they are of course still relevant for thermodynamic properties such as the specific heat.

C. Valence bond theory

We now address the important issue of why the $S \rightarrow S-1$ contribution to the spectral weight is so small. We will argue that this is, in fact, consistent with our scenario of the low-energy excitations being due to effectively isolated magnetic moments. To illustrate this point, Fig. 12 shows valence bond states for a six-site cluster with ground-state spin $S=1$. The state in (a) is constructed as an approximate ground state based on the notion that triplet bonds should be predominantly located in regions of sublattice imbalance. This cluster has two dangling spins, which we take at maximum separation. For the two singlet bonds, we construct a symmetric combination (which corresponds to the true ground state of the Heisenberg model on the four sites in isolation). It is now natural to assume that the lowest excitation corresponds to converting the triplet bond into a singlet, as shown in (b). Diagonalizing the Hamiltonian exactly, we find that these simple states indeed are good approximations to the eigenstates; the overlap of (a) with the true ground state is 0.814 while the overlap of (b) with the lowest $S=0$ state (which is the lowest excited state) is even larger at 0.973. On the other hand, if we act with $S^z_{\pi, \pi}$ on state (a), as explained above with the spin operator written in the form [Eq. (40)], we obtain the state shown in Fig. 12(c). This state mixes $S=0$ and 2 states, and its overlap with the actual lowest $S=2$ state is 0.789. The overlap of (c) with the approximate $S=0$ state (b) is exactly 0 and the overlap with the exact lowest singlet also vanishes. In the case of (b), (c) overlaps, it is immediately clear that it is zero because of their different states of the long bond. The states also differ in the quantum number related to a 180° rotation of the cluster; (b) is odd and (c) even under this symmetry transformation. The true ground state is also odd, which explains why the overlap with state (c) is exactly 0. This latter property is of course particular to this symmetric six-site cluster. In general, for a less symmetric larger cluster with two dangling spins, we

would expect some small overlap between $S_{\pi,\pi}^z|\Psi_S\rangle$ and the lowest $S-1$ state because the triplet will not be exactly localized at only two sites.

Based on the above example, we can understand that, in general, $S>0$ ground states contain some triplet bonds connecting nonbipartite sites. The lowest excitation should normally have spin $S-1$ and closely correspond to converting one triplet bond into a singlet. On the other hand, acting with the spin operator one obtains a linear combination of $S-1$ and $S+1$ states with an additional triplet bond, and the overlap of the $S-1$ component with the low-energy states with this spin is low (because of the differing singlet/triplet state of one nonbipartite bond). The lowest $S-1$ excitation should thus be very similar to the excitations we have argued for in the case of the $S=1$ excitations of a singlet ground state, which essentially corresponds to promoting a long singlet (between two moments, which can be located far away from each other) into a triplet. For an $S>0$ cluster we instead demote a long triplet bond into a singlet. This similarity also suggests that the true dynamic exponent (giving the scaling of the lowest energy, not the dominant spectral weight) in the case of $S>0$ clusters should be the same $z\approx 2D_f$ that we have found for the $S=0$ clusters.

V. BILAYER MODEL AT p^*

Our hypothesis for the low-energy excitations is that they are due to effectively unpairable spins on the percolating cluster. To test this hypothesis further, we consider a case where there are no such spins; the bilayer Heisenberg antiferromagnet with “dimer dilution,” i.e., two identical clusters coupled through a nearest-neighbor interlayer coupling $J_{\perp}=gJ$. The Hamiltonian for this system was already written down in Eq. (2). Its static properties were studied in Refs. 1–4. The percolating cluster remains ordered at $T=0$ when the coupling ratio $g\leq 0.1$, whereas for larger interlayer couplings the cluster is quantum disordered. Here we consider $g=0.01$; well inside the ordered regime. One might then expect the quantum-rotor picture to be valid, as has been argued also based on field theoretical considerations⁵ and, thus, the dynamic exponent should be $z=D_f\approx 1.89$. Scenarios involving “fractons” are also possible.¹⁵

Figure 13 shows scaling results of the kind we previously discussed for the single layer. The peak of the probability distribution of the bound Δ^* for different cluster sizes L (the largest cluster of diluted $L\times L$ lattices) coincides when scaled with L^z and $z\approx 1.7$. This exponent is slightly smaller than D_f but considering statistical uncertainties of several percent and effects of subleading size corrections, $z=D_f$ is plausible, in contrast to $z\approx 2D_f$ in the single layer. Note that the data in Fig. 13(a) do not collapse onto a single curve as clearly as in the single-layer plots 4 and 5. The scaled gap distributions instead appear to become narrower with increasing L . This may be due to self-averaging following from the global nature of quantum-rotor excitations. The local-gap distribution (not shown here) also does not scale well with L .

VI. SINGLE LAYER AWAY FROM THE PERCOLATION POINT

An interesting question is whether the small energy scale of the single-layer clusters at p^* survives also away from the

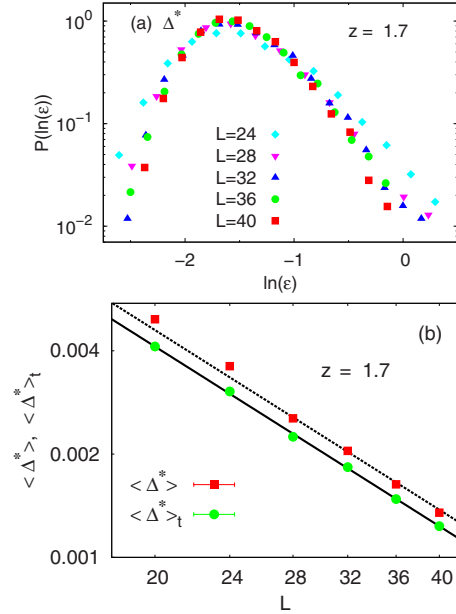


FIG. 13. (Color online) Properties of the gap upper bound Δ^* for dimer-diluted bilayer systems at interlayer coupling $g=0.01$ at the percolation point. (a) shows the scaling of the full probability distribution with $z=1.7$ while (b) shows the size dependence of the average and typical values along with lines corresponding to the asymptotic behavior with $z=1.7$.

percolation point. We here examine $L\times L$ systems diluted at $p<p^*$, again studying the largest cluster for each dilution realization (which now is two dimensional; $\langle n \rangle \sim L^2$). We only consider clusters with ground-state spin $S=0$.

Figure 14 shows results for the gap upper bound at $p=0.3$. For the largest few sizes the data are consistent with power-law scaling corresponding to $z=D=2$ (with a statistical error of $\approx 10\%$); very different from the behavior at p^* . Given our scenario for the excitations exactly at p^* , the much smaller z away from p^* is either an indication of the moment regions not existing or their mutual effective couplings (or their couplings to the rest of the cluster) being much stronger, thereby invalidating the picture of an effective low-energy subsystem. We still expect regions of sublattice imbalance away from p^* , as we will discuss further in the next section. It may not be surprising, however, that the moments associated with these are not weakly coupled because for any $p<p^*$ the largest cluster has a finite spin stiffness (also in the thermodynamic limit), whereas exactly at p^* the stiffness vanishes (although the cluster is still ordered).⁹ The order is thus much more robust and as a consequence all the effective moments at $p<p^*$ may be locked to the global Néel vector and cannot be regarded as weakly coupled semi-independent degrees of freedom. We will discuss this further in Sec. IX.

For systems very close to the percolation point, $p^*\approx 0.407$, one cannot expect to detect differences from the behavior exactly at p^* . For the smaller cluster sizes at $p=0.3$ we can observe in Fig. 14 what is likely a crossover behavior from the behavior at p^* to the asymptotic scaling behavior at $p=0.3$. The effective exponent below sizes $L\approx 20$ is smaller than the value we found at p^* but, on the other hand, $p=0.3$ is already quite far away from p^* and it is

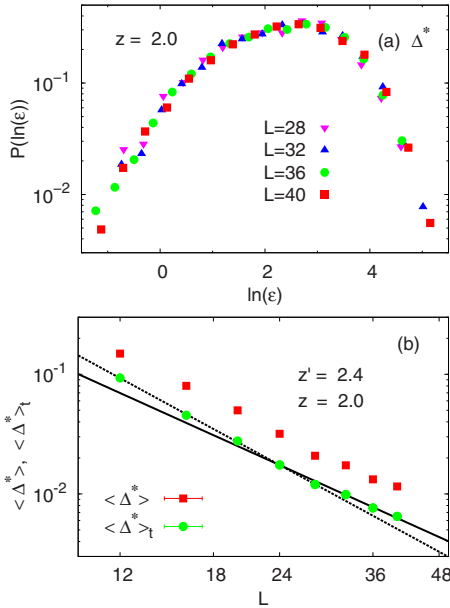


FIG. 14. (Color online) Scaling properties of Δ^* of single-layer clusters at dilution fraction $p=0.3$. For $L \geq 28$, the distribution can be collapsed with dynamic exponent $z=1.8$ as shown in (a). For smaller sizes, there is a crossover behavior, as shown in (b) for the average and typical Δ^* . The two lines correspond to $z=2$ (a possible asymptotic value) and $z'=2.41$ (a pseudoscaling exponent in a crossover regime).

not surprising that a different behavior obtains here. Closer to p^* we expect data for small sizes to scale with $z \approx 2D_f$ but to observe clearly this scaling, followed by a crossover to $z=D=2$, would require larger clusters than we can access currently.

It should be noted that the results discussed here (and those for the bilayer in the previous section) do neither prove that the mapping to quantum rotors holds for $p < p^*$ (and in the bilayer at p^*) nor that the dynamic exponent exactly equals $D=2$ (or D_f). For fracton excitations, one would expect $z \neq D_f$ (but close to D_f).¹⁶ It would therefore be useful to determine z for the single layer at $p < p^*$ and the bilayer at p^* to higher precision, which, however, is a very demanding task that we leave for future studies.

VII. CLASSICAL DIMER-MONOMER MODEL

In the mapping of a quantum antiferromagnet onto a quantum-rotor model,¹¹ one assumes that there is local antiferromagnetic order on some length scale Λ . A subsystem i of the system, of length Λ , is then replaced by a quantum rotor \mathbf{L}_i , which can reproduce the “Anderson tower” of low-energy states of different total spin S (which the subsystem would exhibit in isolation). The rotors for all the subsystems are then coupled in a way consistent with the expected dominant fluctuations and symmetries of the system. For such a mapping to produce the correct physics, the subsystems should consist of an even number of spins, arranged in such a way that their ground state, in isolation, is a singlet. If the system geometry does not allow for such a decomposition, the situation will be more complicated. The question is then:

How can one decompose the system into quantum rotors and “left-over” spins in a well-defined way, which maintains the salient features of the disordered clusters?

The smallest unit for which a local quantum rotor can be considered in a hypothetical mapping is a dimer consisting of two nearest-neighbor spins, which in isolation has a singlet ($l=0$) ground state and a triplet ($l=1$) excited state. This corresponds to a quite severely truncated rotor tower but the local cutoff should not matter for the low-energy physics of the coupled system. We have already discussed the fact that a disordered cluster cannot normally be fully decomposed into such dimers, as there would in most cases be some dangling spins (or, more generally, regions of imbalance in the sublattice occupation numbers) left over after the cluster has been maximally covered with close-packed dimers. If we consider larger subsystems, there will be similar problems, i.e., not all subsystems will have singlet ground states in isolation. We will here proceed to investigate the geometric decomposition of the system into nearest-neighbor dimers and left-over monomers.

In a standard classical dimer model,³⁴ a dimer corresponds to two connected nearest-neighbor sites, here on a square lattice. The statistical-mechanics problems correspond to counting all the dimer coverings. In a dimer-monomer model,³⁵ there are also some unpaired sites present and the counting now includes all possible dimer and monomer configurations; normally at a fixed density of monomers. In the case at hand here, we investigate disordered clusters and we want to maximally cover the clusters with dimers. There will then typically be some left-over monomers that cannot be paired. For a given cluster, we want to sample dimer-monomer configurations with the smallest possible number of monomers. We are interested in the spatial distribution of monomers, which provides us with a concrete quantitative measure of “sublattice imbalance.” We want to identify the regions of sublattice imbalance and investigate the size distribution of these regions.

Here we consider clusters constructed on $L \times L$ lattices, with, as before, only the largest cluster found in each realization included in the statistics. In Monte Carlo sampling of the dimer-monomer configurations on these clusters, we start with an arbitrary configuration, e.g., one containing only monomers. The updating scheme is illustrated in Fig. 15. In (a), when two monomers are located next to each other, they are annihilated and form a dimer. Dimers and monomers can be updated together according to the two moves shown in (b). We can also break a dimer into two monomers, as in (c). One of the monomers is then moved, together with dimers as in (b), until it encounters a monomer (which can, but does not have to, be the same as the one it was originally paired with), together with which it again can be combined to form a dimer as in (a). This is an efficient way to update parts of the cluster where there are no monomers (other than the two introduced for the purpose of the update). This simulation process will eventually converge to a state with the minimum number of monomers for a given cluster because the monomer annihilation process (a) is always carried out when possible. Whenever two monomers are created, they will eventually be annihilated. Our model is therefore also an aggregation model for dimers.

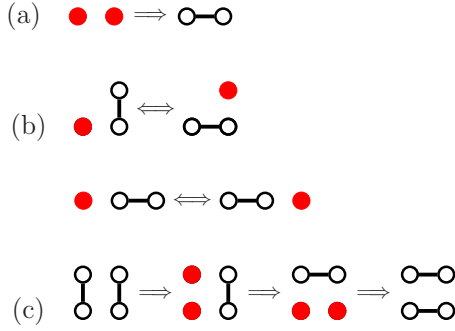


FIG. 15. (Color online) Updating processes used in Monte Carlo sampling of the classical dimer-monomer aggregation model. (a) is the annihilation of two monomers, leading to a dimer. (b) shows the two elementary monomer-dimer moves. In (c), a monomer pair is temporarily created out of a dimer. One of the monomers is then moved until it can be annihilated with another monomer. A large number of dimers can be changed in such “loop updates.”

For a given cluster generated on an $L \times L$ lattice, after a long equilibration to make sure that the minimum monomer number has been reached, we collect statistics. One quantity of interest is the average monomer density for each site. Most of the sites never have any monomers. We define a “moment” as a region consisting of S_m sites to which one or several monomers are confined. By definition, a monomer inside such a moment cannot move to a different moment through the Monte Carlo processes. In addition, the moments consist only of sites on the same sublattice because an individual monomer only moves on a given sublattice, as in Fig. 15(b). Two moments on different sublattices cannot have any sites that are nearest neighbors because then two monomers in these different regions could become adjacent and annihilate each other.

Keeping track of the moment regions and their sizes involves straightforward book keeping and we just proceed to discuss results. Figure 16 shows the size distribution of the moments both at the percolation point and away from it, at $p=0.3$. For small moment sizes S_m , the distribution is close to a power law, especially at $p=0.3$, but there is a crossover to a clearly exponential decay for large S_m . The distribution can be fitted well with the form $e^{-S_m/\sigma}$, with $\sigma \approx 42$ and ≈ 300 at p^* and $p=0.3$, respectively. The average moment size $\langle S_m \rangle$ computed as a sum over all the sizes is smaller; $\langle S_m \rangle \approx 16$ at p^* and ≈ 47 at $p=0.3$. In the figure, the largest cluster sizes are much larger than $\langle S_m \rangle$ and σ , and the curves for the largest L overlap almost completely.

These calculations prove that the notion of local sublattice imbalance is well defined and quantifiable. Finite moment regions exist both at and away from the percolation point. In the next section, we will present result from valence bond quantum Monte Carlo simulations in the triplet sector. We will also look at the spatial distribution of the monomers in the classical dimer-monomer model and compare it with the distribution of the triplet in the lowest excitation of the actual quantum spin model.

VIII. SPATIAL DISTRIBUTION OF SINGLET-TRIPLET EXCITATIONS

As discussed in Sec. II C, the valence bond projector QMC method offers us the possibility to examine the lowest

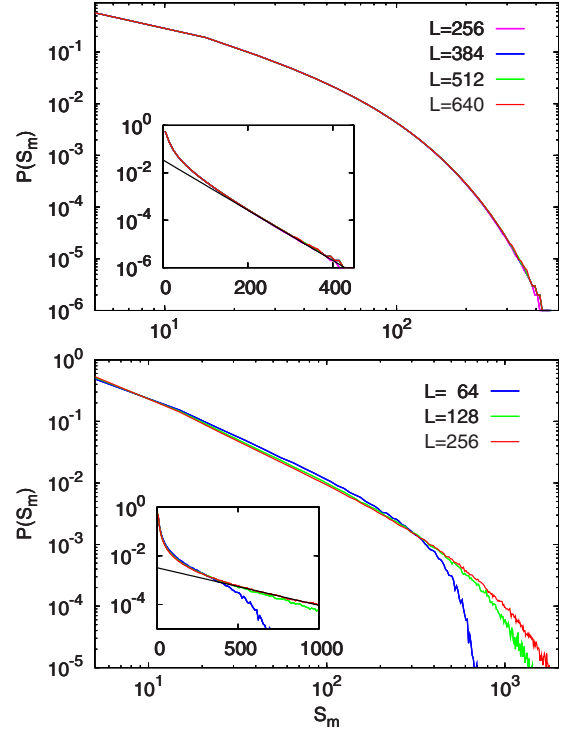


FIG. 16. (Color online) Probability distribution of the moment size of the classical dimer-monomer model at the percolation point p^* (top panel) and at $p=0.3$ (bottom panel) graphed on a log-log scale. Hundreds of realizations of the largest cluster on $L \times L$ lattices were used. For large L the distributions collapse onto a single curve, reflecting a finite typical moment size. The average moment size is $\langle S_m \rangle = 16$ at p^* and 47 at $p=0.3$. The asymptotic form of the probability distribution for large clusters is $\propto e^{-S_m/\sigma}$, as shown in the insets using a semilogarithmic scale.

triplet state in a unique way. In a disordered system, the spatial distribution of the triplet bond gives a very direct measure of the extent to which different parts of the system are affected when exciting a cluster with $S=0$ ground state to its lowest $S=1$ state. An example of the triplet density for a very small cluster was already presented in Fig. 1. It should be noted that the statistics of the singlet bonds is also affected by the presence of a triplet bond and, thus, just examining the properties of the triplet bond does not give a complete picture of the excitation. However, if a large region of the system has no (or very low) average triplet density, then the singlets of that region should also not be much affected. The spatial distribution of the triplet should therefore provide a valid measure of the tendency (if any) of the triplet excitation to localize.

We study the site-dependent triplet density $\rho_i = \langle n_t(i) \rangle$, where the triplet occupation number $n_t(i)$ is defined such that if a triplet bond connects sites i and j , then $n_t(i) = 1$ and $n_t(j) = 1$ while $n_t(k) = 0$ for all other sites k . In addition to visually examining the triplet density for representative individual clusters, it is also useful to have a quantitative measure of localization. For this purpose, we use the inverse participation ratio (IPR) corresponding to the triplet density,

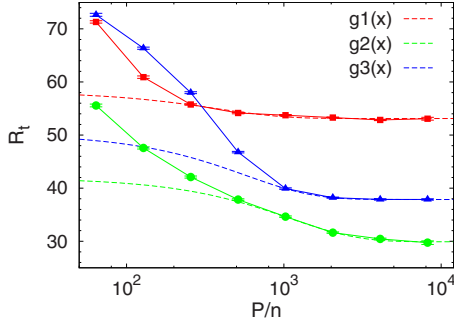


FIG. 17. (Color online) (a) Examples of the convergence of the average triplet IPR for three individual clusters as a function of the projection power, here normalized by the cluster size as P/n . The clusters were generated on 26×26 lattices. The dashed curves are of the form $a + be^{-cP/n}$, with a, b, c adjusted to fit the last few (large P/n) points.

$$R_t = \frac{\left(\sum_{i=1}^n \rho_i \right)^2}{\sum_{i=1}^n \rho_i^2} = \frac{4}{\sum_{i=1}^n \rho_i^2}. \quad (42)$$

This quantity characterizes the number of sites involved in a triplet excitation and can be averaged over cluster realizations. Two extreme cases can help to clarify the meaning of R_t ; if the triplet is completely localized on only two sites, then $R_t=2$ while if it is equally spread out over all the sites of an n -site cluster, then $R_t=n$. We will study the dependence of $\langle R_t \rangle$ on the cluster size.

In a projector method based on a power H^P , one converges to the lowest state in a given symmetry sector when the power P of the Hamiltonian is sufficiently high. For an n -site cluster, one would expect that the P required for convergence scales as n or worse. This can be seen if we compare with an alternative projection method—the imaginary-time evolution $e^{-\beta H}|\Psi\rangle$ of the trial state. Here β is analogous to an inverse temperature; starting from a state at some “temperature,” we “cool it” by increasing β . A better trial state corresponds to a lower initial temperature. For large β , the dominant power \tilde{P} in a Taylor expansion of $e^{-\beta H}$ is $\tilde{P} = \beta|E_0|$, where E_0 is the ground-state energy, which is proportional to the cluster size n . Thus, if we project with just a fixed power P of H , we would get essentially the same result if $P \approx \tilde{P} \propto \beta n$. The energy scale of the excitations decrease with increasing n (very quickly so in the problem under consideration here, because the dynamic exponent is large), and we should therefore expect to need larger β for larger n . Thus, in the fixed-power scheme, the P required for convergence should increase as some power (larger than one) of n .

We show examples of the convergence of the IPR for three different clusters in Fig. 17. The large fluctuations in the finite-size gap, discussed in Sec. III, naturally also imply large variations in the convergence rate of the triplet IPR (which is governed by the gap between the first and second triplets, which also exhibits large fluctuations). As explained in Sec. II C, we are restricted to P for which the triplet sur-

vival probability in the projection is reasonably large. In order to ensure that the results truly reflect the lowest excitation for each cluster, we carry out extrapolations to infinite P using a simple exponential form, as explained in the caption of Fig. 17. The fluctuations of the disorder averaged $\langle R_t \rangle$ are completely dominated by the cluster-to-cluster variations, and we believe that any remaining errors related to the convergence are smaller than the final error bars (based on a few hundred clusters of each size).

We first examine the spatial distribution of the triplets. The triplet density for each site of a typical cluster is shown using a color scale in Fig. 18(b). Here we compare the triplet density with two other calculations—the classical monomer density in (a) and the local gap Δ_i in (c). It is apparent that the triplet is concentrated to a relatively small fraction of all the sites of the cluster. At the same time, the affected sites form groups that are spread out over the cluster. This is exactly in agreement with our hypothesis of low-energy excitations involving a number of localized moments. It is also clear from Fig. 18 that the classical monomer density is high wherever the triplet probability is significant. This proves that our measure of sublattice imbalance in terms of classical monomers indeed corresponds very closely to the actual locations affected by excitations. Note also that some sites with high monomer density do not have a high triplet density. This is also expected because the *lowest* triplet excitation should not necessarily involve all of the classical monomer regions. Higher triplet states may involve other subsets of moments. Finally, there is a very good correspondence between regions of low local gaps Δ_i and high triplet density.

Next, we discuss the IPR of the triplet. It is interesting to compare this with the total number of monomers in the classical dimer-monomer model. We therefore also define a classical IPR, as in Eq. (42) but with the triplet density ρ_i replaced by the classical monomer density. Both these IPRs, averaged over several hundred clusters, are shown versus the cluster length L on a log-log scale in Fig. 19. They both scale according to power laws. The classical IPR is consistent with the form $L^{D_f} \sim \langle n \rangle$. In combination with the fact that the individual moment regions are finite, as we showed in the previous section, this is in agreement with our extremal-value analysis in Sec. III B, which relied on the number of effective moments being proportional to n . However, the triplet IPR scales with a smaller power; $\langle R_t \rangle \sim L^\gamma$ with $\gamma=1.39(3)$. Thus, not all the effective moments are involved in the lowest excitation but since the size of the excitation still grows with L these are not localized excitations.

Another important aspect of the valence bond calculation is that the bond lengths also contain information directly pertaining to the nature of the excitations. In Fig. 20 we show the distributions of both the singlet and triplet bond lengths for the cluster shown in Fig. 18. While the triplet bond is typically long, the singlet distribution is strongly peaked for the shortest bonds. We have therefore cutoff more than 90% of the weight in the singlet histogram in order to be able to show the more interesting distribution of long bonds. Every peak in the triplet distribution can be perfectly matched to the distance between two regions (on different sublattices) with a high concentration of triplets/monomers in Fig. 18. This again supports the notion of excitations of

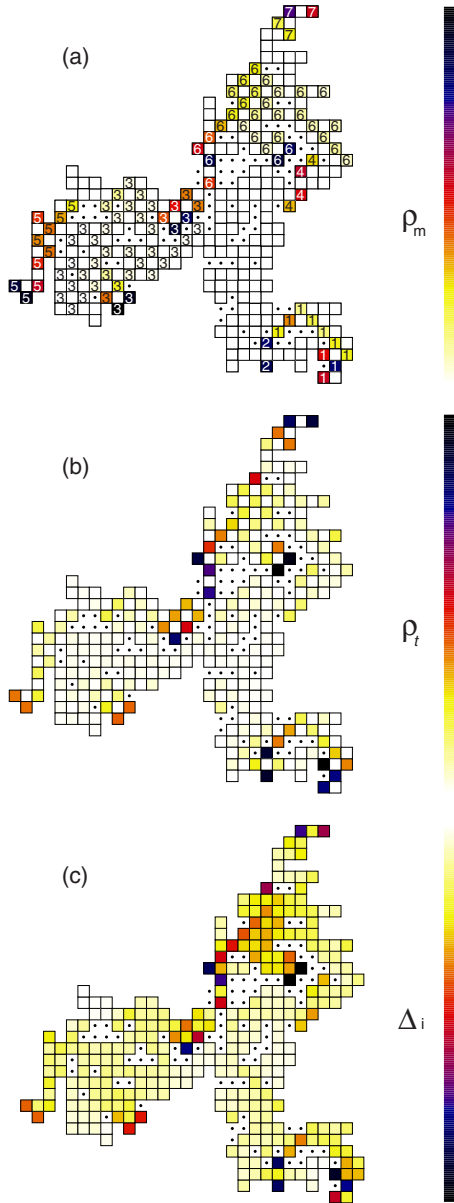


FIG. 18. (Color online) Properties of a typical cluster with 288 sites; (a) the classical monomer density, (b) the triplet density, and (c) the local gap estimate Δ_i . All quantities are shown on a color scale ranging from the smallest (0 in the case of ρ_t and ρ_m) to the largest value. The absolute values are irrelevant for the purpose of the discussion here. In (a), the numbers inside the squares label the different classical moment regions. The dots indicate empty sites.

weakly interacting effective moments. In the singlet distribution, there are also features corresponding to the same lengths as in the triplet case. This is also what one would expect if the triplet state essentially corresponds to promoting a long singlet to a triplet in a superposition, as discussed in Sec. IV C. The average length of the triplet bond also scales with the cluster size according to a power law, as shown in Fig. 21. This power law, in combination with that for the triplet IPR (Fig. 19) and classical percolation exponents, should be related to the dynamic exponent $z \approx 3.6$. Exactly how is not presently clear, however.

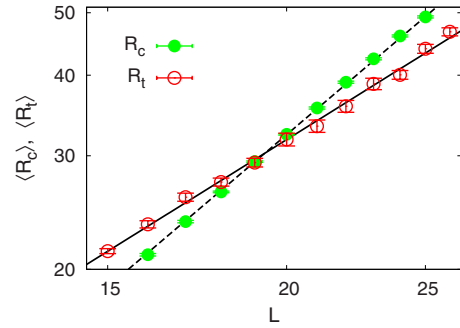


FIG. 19. (Color online) Log-log plot showing the finite-size scaling of the IPR of the triplets (R_t) and the classical monomers (R_c). The lines correspond to scaling L^γ , with $\gamma=1.39(3)$ (based on a line fit) for R_t and $\gamma=D_f$ for R_c .

IX. SUMMARY AND DISCUSSION

To summarize, we have discussed several calculations aimed at elucidating the quantum dynamics of the $S=1/2$ antiferromagnetic Heisenberg model on randomly diluted clusters. Quantum Monte Carlo simulations in combination with sum rules show that the low-energy excitations at the percolation point are described by an unexpectedly large dynamic exponent; $z \approx 3.6 \pm 0.1 \approx 2D_f$, where $D_f=91/48$ is the fractal dimension of 2D percolation. Using extremal-value statistics, we were able to relate z and two exponents characterizing the probability distribution of local gaps (an exponent a governing the size dependence and ω describing the distribution of small gaps), according to Eq. (38). This kind

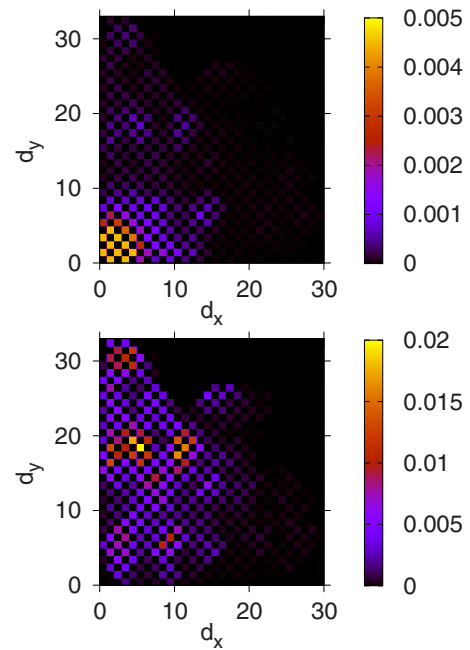


FIG. 20. (Color online) Probability distribution of the length (d_x, d_y) of the singlet (top panel) and triplet (bottom panel) bonds for the cluster in Fig. 18. The singlet distribution is strongly peaked at short bonds and we have therefore cutoff the corresponding peak in the low left corner of the histogram. The remaining weight is 9% of the total.

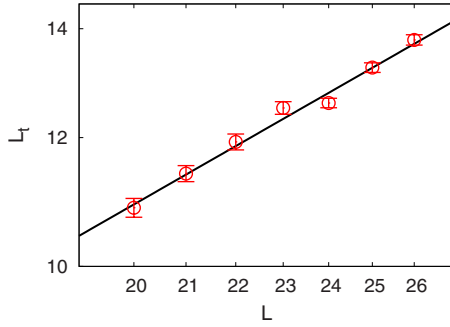


FIG. 21. (Color online) Size dependence of the average length of the triplet bond on $L \times L$ clusters. The line corresponds to a power-law divergence $L_t \sim L^\alpha$, with $\alpha = 0.81 \pm 0.03$.

of scaling indicates that the excitations involve effective localized finite magnetic moments, which interact through the remaining, magnetically inert parts of the cluster. This is also confirmed directly by imaging the spatial distribution of the triplet excitations in the valence bond basis, where the triplet state can be described in terms of a pair of spins forming a triplet in a “singlet soup” of valence bonds. The triplet bond fluctuates between several isolated regions and its average length scales as a power of the cluster size. The average number of spins affected by the excitation also grows as a power n^β of the system size, with $\beta \approx 0.74$. The excitations are thus localized at multiple moment regions, which are spread out over the cluster. All these results lead to a picture of an effective low-energy system consisting of a network of globally entangled local moments, where the moments correspond to regions of sublattice imbalance.

We have introduced a quantitative measure of sublattice imbalance, in terms of a classical dimer-monomer aggregation model. Monte Carlo simulations of this model show that the monomers form isolated finite regions and the number of such regions scales linearly in the cluster size n . Sites with a high triplet concentration coincide very well with high monomer density, confirming directly that sublattice imbalance in the Heisenberg model is associated with the formation of weakly interacting effective moments.

We have also shown that when two identical clusters are coupled in a bilayer, with a small interlayer coupling J_\perp (smaller than the value at which the long-range order vanishes¹), the low-energy excitations change dramatically. A finite-size scaling analysis for clusters with $J_\perp/J = 0.01$ show a much smaller dynamic exponent, $z \approx D_f$, than for the single-layer clusters. There is no sublattice imbalance in this “dimer-diluted” bilayer model and the results therefore provide additional evidence for the important role played by effective moments at imbalanced regions in the single-layer clusters.

The result $z \approx 3.6$ was obtained by studying clusters in which the sublattices are balanced globally, i.e., the ground-state spin is $S=0$. We have also pointed out that for clusters with global imbalance in the sublattice occupation (leading to $S > 0$), the dynamic structure factor has spectral weight predominantly arising from the $S \rightarrow S+1$ channel while there is very little weight in the $S \rightarrow S$ and $S \rightarrow S-1$ channels (apart from the elastic $S \rightarrow S$ weight). Experiments directly probing

the inelastic spectral weight, e.g., neutron scattering and nuclear magnetic resonance, should be dominated by the $S \rightarrow S+1$ channel and S should be typically large ($\propto \sqrt{n}$) for random clusters. For this situation our sum-rule method gives a smaller effective dynamic exponent, $z \approx 1.5D_f$, than for the $S=0 \rightarrow 1$ excitations of globally balanced clusters. The lowest-energy excitations, which are in the $S \rightarrow S-1$ channel, are not accessible with the sum-rule approach. We have argued, based on an analysis of approximate (variational) valence bond states, that their energy should scale with the same $z \approx 3.6 \approx 2D_f$ as in the case of $S=0 \rightarrow 1$ excitations.

There have been attempts previously to determine the dynamic exponent of the diluted Heisenberg model based on quantum Monte Carlo calculations. Yu *et al.*⁶ studied the temperature dependence of the correlation length and concluded that it scales in a way consistent with $z=D_f$ at the percolation point. However, the scaling assumption was one corresponding to quantum criticality, which may not apply because the percolating cluster at $T=0$ does not have quantum-critical fluctuations in the sense of power-law decaying correlation functions. A similar treatment of the clean 2D Heisenberg model would fail to give $z=D$ (which is not a quantum-critical exponent but one characteristic of the quantum-rotor excitations of the Néel state) because the correlation length diverges exponentially as $T \rightarrow 0$.³⁶

We have here focused exclusively on the dynamics of the percolating cluster. In order to relate the results quantitatively to specific experiments, one should include the contributions from all clusters. The cluster distribution is given by classical percolation theory,¹³ which can be combined with the finite-size scaling properties that we have found here for the distributions of the local and smallest gaps. We have also not discussed the consequences of our $T=0$ results for the $T > 0$ behavior. This is of course also an important experimental issue and will be interesting to consider in future studies.

Moving away from the percolation point p^* , our calculations show that the dynamic exponent of the single layer is $z \approx 2=D$. However, the classical dimer-monomer model has finite localized monomer regions also away from the percolation point. This suggests that the change in the spin dynamics upon moving away from p^* is related to the effective interactions between the moment regions, not the disappearance of the moments. Such a qualitative change in the interaction aspects of the moments is not completely unexpected since the spin stiffness of the percolating cluster at p^* is strictly zero in the thermodynamic limit^{9,37,38} (although the cluster is ordered), whereas it becomes finite (according to a power law) away from the percolation point. The more robust cluster order for $p < p^*$ should qualitatively change the effective interactions between distant monomer regions, likely locking all of them to the global Néel vector (which is the case for a single moment in a 2D system^{17,18}). The effectively independent nature of the magnetic moments exactly at the percolation point (and the very weak interactions between them) are thus intimately related to the fractal structure and related vanishing spin stiffness of the network connecting the moment regions. We presented some results showing the crossover from scaling controlled by the percolation point to 2D behavior.

In spite of the close agreement with the dynamic exponent expected based on the quantum-rotor mechanism⁵ for the single layer away from p^* and the bilayer at p^* , it is still not certain that the lowest-energy excitations in these systems are quantum-rotor states. Over the years there have been considerable efforts to understand the dynamics of various randomly diluted systems close to and at the percolation point. The fracton has been introduced as a generic excitation which develops out-of-plane waves (e.g., spin waves for an antiferromagnet) for a translationally invariant system upon dilution.¹⁵ Numerical calculations based on spin-wave theory show that the dynamic exponents for fractons in the 2D percolating antiferromagnet is very close to D_f .¹⁶ This calculation does not properly account for the vanishing spin stiffness of the percolating cluster at p^* and the existence of localized moments, but it may still be valid close to the percolation point (where a finite stiffness develops). It is possible that the dynamic exponents $z \approx D=2$ and $z \approx D_f$ that we have obtained here for the single layer with $p < p^*$ and the bilayer at p^* , respectively, are due to fractons, not quantum rotors. However, exactly at the percolation point, the physics of the globally entangled local moments that we have discussed here is clearly different from fractons (which can exist in systems that do not have any objects corresponding to localized moments) and the value of the dynamic exponent is twice that expected based on fractons.¹⁶ It is thus possible that several types of excitations coexist at and close to the percolation point; quantum rotors, fractons, and the globally entangled moment excitations.

One may still be able to describe the low-energy physics of the system away from the percolation point as a network of weakly interacting moments but now in the presence of a staggered field mimicking the coupling to a common Néel vector (i.e., the sign of the field depends on which sublattice a moment is associated with on the original lattice). The strength of the effective staggered field (which for a finite cluster should be allowed to have a fluctuating direction as well¹⁸) should increase upon moving away from the percolation point (being 0 at p^* , due to the vanishing spin stiffness—the energy scale of twisting the Néel order globally). Most likely, even an infinitesimal field will asymptotically (for large clusters) change the dynamic exponent.

The role of effectively isolated spins in the formation of long-range order⁹ on the percolating cluster has been pointed out by Bray-Ali *et al.*^{37,38} 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 “floppy” fractal cluster (one with vanishing spin stiffness) can order at $T=0$. This picture seemingly contains some of the ingredients of our entangled moments picture. However, the same ordering mechanism was argued to apply both to antiferromagnets and systems of coupled quantum rotors, whereas we have shown here that the bilayer (which should correspond more closely the coupled rotor system since there is no sublattice imbalance) and the single layer behave dramatically different. Since the excitations of the single-layer cluster are also much lower in energy than the quantum-rotor states considered in previous

discussions of the dynamic exponent,⁵ a theoretical treatment within a quantum-rotor picture is clearly not adequate. In Refs. 38 and 39 the excitations of the diluted system were analyzed using spin-wave theory but this method also does not capture the significance of almost isolated moments and their long-range global entanglement, and no unusually low-energy scale was discussed.

In field-theory language, the dangling spins, or regions of sublattice imbalance, that we have discussed here correspond to uncompensated Berry phases.¹¹ Although it is quite clear that these should exist in diluted quantum antiferromagnets, how to properly take them into account in analytical calculations for these systems is not well understood. To our knowledge, the resulting globally entangled moments excitations that we have argued for here have not been discussed previously in the literature. The effective low-energy system is similar to the random antiferromagnet considered by Bhatt and Lee,⁴⁰ and also by Sachdev and Ye.⁴¹ However, there is an important difference in that the nearest-neighbor interactions in our system are not frustrated. An effective low-energy Hamiltonian should then also not be frustrated.

The Bhatt-Lee calculation⁴⁰ was focused on the thermodynamic properties and did not address the dynamic exponent. The method applied was a generalization of the strong-disorder renormalization (singlet decimation) scheme by Ma *et al.*,⁴² which has been applied to numerous random antiferromagnetic Heisenberg systems.^{33,43,44} It would be interesting to apply this method also to the diluted clusters. However, there is a technical problem in doing this directly since the decimation scheme is based on random couplings (successively eliminating the strongest coupled spin pair and including their remaining effects as modified couplings calculated perturbatively), whereas in the diluted system all couplings are the same. It may be possible to carry out a decimation procedure by eliminating strongly *correlated* spins, instead of strongly *coupled* ones. The correlations could be computed perturbatively based on regions of a small number of spins or using quantum Monte Carlo simulations. This way, one could study the renormalization flows of the correlations and how they relate to the sublattice imbalance that we have quantified here in terms of the classical dimer-monomer systems. The final stages of the decimation procedure should lead to bonds (entanglement) between the sites on which our projector QMC calculations give a high triplet probability. However, we have shown that there are large fluctuations in the long bonds (singlet as well as triplet) and it is therefore clear that the scheme cannot asymptotically give the correct ground state and low-energy excitation in terms of a single bond configurations. In one dimension, the final “random singlet state” is known to be asymptotically exact,⁴³ in the sense that a single bond configuration is a good representation of a superposition including fluctuations around this reference state.⁴⁵ With large fluctuations of long valence bonds among many moments in the percolating clusters, it seems unlikely that a single reference configuration would be a good approximation in this case. It would still be interesting to investigate the flow of the renormalized coupling distribution.

To go further in developing an understanding of the excitations of the weakly interacting effective moments, instead

of working with the full percolating clusters it may be better to explicitly construct the effective low-energy Hamiltonian we have discussed here. While the geometrical locations of the moments could be obtained using the classical dimer-monomer model, the effective couplings are more challenging. One approach would be to just study a bipartite network of spins with some suitable form of the interactions (which should be nonfrustrated, with antiferromagnetic couplings between sublattices and ferromagnetic intrasublattice couplings). In principle the spins should have mixed S . In one dimension such a system is known to have different properties than the random $S=1/2$ chain with only antiferromagnetic couplings.⁴⁴ The effective system could be studied with the methods used here, as well as with the strong-disorder

decimation scheme. Comparing results for the moment network with the dynamic exponents we have extracted here for the full cluster system (and investigating the robustness of the exponents to variations in the couplings) could shed further light on this challenging problem.

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