Emergent Spin Excitations in a Bethe Lattice at Percolation

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We study the spin-1/2 quantum Heisenberg antiferromagnet on a Bethe lattice diluted to the percolation threshold. Dilution creates areas of even or odd sublattice imbalance resulting in "dangling spins" [L. Wang and A. W. Sandvik, Phys. Rev. Lett. **97**, 117204 (2006); Phys. Rev. B **81**, 054417 (2010)]. These collectively act as "emergent" spin-1/2 degrees of freedom and are responsible for the creation of a set of low-lying "quasidegenerate states." Using density matrix renormalization group calculations, we detect the presence and location of these emergent spins. We find an effective Hamiltonian of these emergent spins, with Heisenberg interactions that decay exponentially with the distance between them.

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Introduction.—Quantum spins on percolation clusters [1] provide an ideal test bed for studying the interplay between geometrical disorder and quantum fluctuations. The Hamiltonian for these problems is

$$\mathcal{H} = \sum_{\langle ij \rangle} J \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where $\mathbf{S_i}$ are Pauli spin-1/2 operators and the sum runs over nearest-neighbor occupied sites, and $J > 0$. Theoretical [2–5] and experimental [6] studies of quantum spins on diluted square lattices have focused on the question of whether or not long range order survives up to the classical percolation threshold p_c. A numerical study [4] has settled this question and found long range order to be robust to quantum fluctuations, surviving all the way up to p_c.

The excitations are less straightforward. For uniform lattices with number of sites N, the lowest energy scale consistent with Néel order breaking a continuous symmetry is $\sim JN^{-1}$, corresponding to a "tower" of states: mixtures of symmetry-broken states that become degenerate in the thermodynamic limit [7–9]. However, a quantum Monte Carlo study by Wang and Sandvik [10] discovered a somewhat "anomalous" finite size scaling of the spin gap Δ_{low}: $\Delta_{\text{low}} \approx N^{-2}$ (for clusters with a singlet ground state) or $\Delta_{\text{low}} \approx N^{-1.5}$ (for generic clusters, most with a non-singlet ground state). A strong correspondence was shown [10] between these low-lying states and places on the cluster where there is a local imbalance between the number of even and odd sites. It was conjectured that, in each such place, a spin degree emerges which is effectively decoupled from the antiferromagnetic order and hence was called a "dangling spin."

The goal of this Letter is to characterize the dangling-spin degrees of freedom numerically, relating their nature to the local geometry of the cluster, and to explain the observed low-energy spectrum in terms of mediated interactions between dangling spins. Our Hamiltonian is (1) on clusters obtained by randomly diluting the Bethe lattice of coordination 3 at its percolation threshold, $p_c = 1/2$ (see examples of small clusters in Fig. 1). The lack of loops in the Bethe lattice is conducive for using the density matrix renormalization group (DMRG) [11] algorithm, as adapted to generic tree graphs [12], to obtain ground and (some) excited states.

In the rest of this Letter, we first show that a typical percolation cluster's spectrum has a clearly separated low-energy component, with a multiplicity consistent with the expected number of weakly coupled spin-1/2 (sometimes spin-1) dangling spins. We next show that each dangling spin is somewhat delocalized over a few sites: on the one hand, we model it as an unpaired spin in a dimerized background to predict the dangling spin's nature from the local geometry; on the other hand, by processing spin

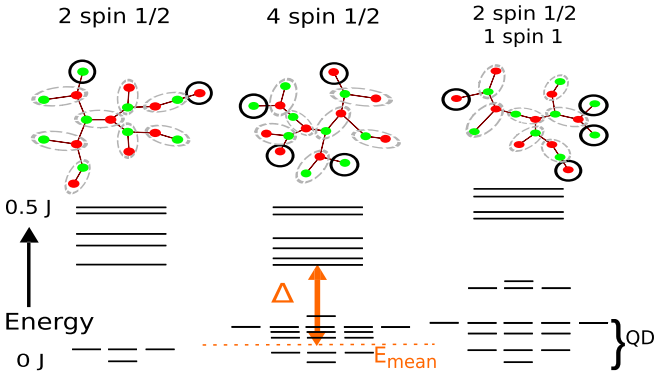

FIG. 1 (color online). Three different percolation clusters (all of the same size $N = 18$) are shown with their corresponding low-energy spectra. The red (dark) and green (light) circles indicate even and odd sites. The broken dashed lines show dimer coverings which serve as a heuristic to locate the "dangling spins" (circled with thick black lines). Energy spectra for each of the clusters show low-lying quasidegenerate (QD) states separated from the continuum by an energy scale Δ. σ_{QD} (not shown) is a measure of the spread of QD energies.

expectations we obtain the explicit "localized state wave function" for each dangling spin. Finally, for each cluster we construct the effective Hamiltonian of the emergent dangling spins, consisting of pairwise, unfrustrated exchange interactions decaying exponentially with separation, mediated by the background of almost dimerized spins on the balanced parts of the cluster; this accurately reproduces the details of that cluster's low-energy spectrum.

Exact correspondence between dangling spins and low energy spectrum.—We carried out DMRG calculations for several hundred balanced clusters (i.e., having an equal number of even and odd sublattice sites) [13] for sizes up to $N = 100$, targeting multiple excited states in the low-energy spectrum. Since the number of low-energy states was found to increase rapidly with an increase in the number of dangling spins, we restricted our analysis to the case of four dangling spins [14].

In a typical percolation cluster, we observed a distinct set of low-lying energy levels we shall call "quasidegenerate" (QD) [15] since (we claim) they would be exactly degenerate in the limit that the dangling spins are fully decoupled from the rest of the sites. The QD states are separated from the continuum of higher energy states by a finite size gap we call Δ (specifically defined as the difference between the mean of QD levels and the lowest non-QD level). The set of QD states is identified by looking at the difference in energies of consecutive states up to the quantum rotor excitation and finding the pair of states with the largest gap. The lower energy state in this pair and all states below that make up the QD spectrum [16]. The energy scale characterizing the spread of the QD states σ_{QD} is defined to be the standard deviation of the QD energies from their mean value. The ratio $r = \langle \sigma_{\mathrm{QD}}/\Delta \rangle$ (where $\langle ... \rangle$ indicates an average over disorder) was found to be small (for example, $r = 0.17 \pm 0.1$ for $N = 50$), justifying our notion of a separation of scales.

Figure 1 also shows a striking correspondence between the number of low-lying QD states $\mathcal{N}_{\mathrm{QD}}$ and the number of dangling spins n_d on the percolation cluster. We find that $\mathcal{N}_{\mathrm{QD}} = 2^{n_{1/2}} 3^{n_1}$, where $n_{1/2}$ and n_1 are integers and $n_{1/2} + 2n_1 = n_d$. Our interpretation of this multiplicity is that $2n_1$ of the dangling spins pair up to form a moment with spin 1, while the others remain as spin-1/2 degrees of freedom. There is thus a one-to-one correspondence between the low-energy (QD) eigenstates and the Hilbert space of the posited emergent spins. We used an algorithm (described later) that relies only on the cluster geometry to objectively predict the numbers $n_{1/2}$ and n_1 for each cluster, and verified that their predicted relationship with $\mathcal{N}_{\mathrm{QD}}$ was satisfied in every cluster.

We also directly measured the lowest singlet-triplet gaps Δ_{low} for an ensemble of balanced clusters (for sizes up to $N = 200$ and not constraining the number of dangling spins). Its typical value scales as $N^{-1.9\pm0.1}$, which appears remarkably similar to the scaling previously seen on square lattice percolation clusters [10].

Locating dangling degrees of freedom in real space.—Having established the presence of emergent spin-1/2 and spin-1 degrees of freedom, we now develop two complementary ways of looking at them.

The first is within the framework of a quantum monomer-dimer model. We imagine that the wave function is a product of valence bonds in which the N spins are paired (dimerized) into singlets to the maximum extent possible (optimal configuration). Even when even and odd sites are balanced globally, there remain some uncovered sites, i.e., monomers, due to local imbalances. These are spin-1/2 degrees of freedom and (within this picture) represent the dangling spins. There are multiple ways to optimally place the monomers; the actual wave function is imagined to be a superposition of these ways.

Our geometric algorithm, based on the valence bond framework, finds one element from the set of optimal dimerizations of the cluster and then attempts to find other elements of the set by locally replacing monomers with adjacent dimers. In spirit, this is a "greedy" algorithm which tries to place dimers wherever possible (to obtain an optimal dimerization pattern), working from the outer sites inwards on the cluster.

Given any cluster, there are two operations which cut it down to a smaller cluster or clusters, such that all optimal dimerizations on the smaller cluster(s) are in 1-to-1 correspondence with some of the dimerizations on the larger one. The first operation is that wherever two sites have coordination 1 or 2, we can remove both (given the dimerization on the smaller cluster, just insert another dimer to get the dimerization on the larger one). The second operation is that wherever we find a pair of adjacent sites with respective coordinations 3 and 1 (a "prong"), we can always place a dimer on that pair, which fragments the rest into two subclusters (Fig. 2); a very common special case is the fork [Fig. 2(a)], at which we can arbitrarily choose either side to be the prong. These two operations can be used recursively till only isolated sites remain, each corresponding to one monomer in the original cluster. Furthermore, any other optimal dimerization is accessible from the special one we constructed, by repeatedly exchanging a monomer with an adjacent dimer.

A monomer can thus "hop" to sites on the lattice via such local monomer-dimer rearrangements as shown in Fig. 2(c). Our rule of thumb is that two monomers (of the same sublattice) form a spin 1 moment if and only if they can approach to the minimal separation of two steps [17].

Our second way to capture the spatial nature of a dangling spin degree of freedom starts from the idea that it could be adiabatically connected to an uncoupled spin, analogous to the Landau quasiparticle that is adiabatically connected to a free electron. Thus, our program is to label each emergent spin-1/2 degree of freedom by a

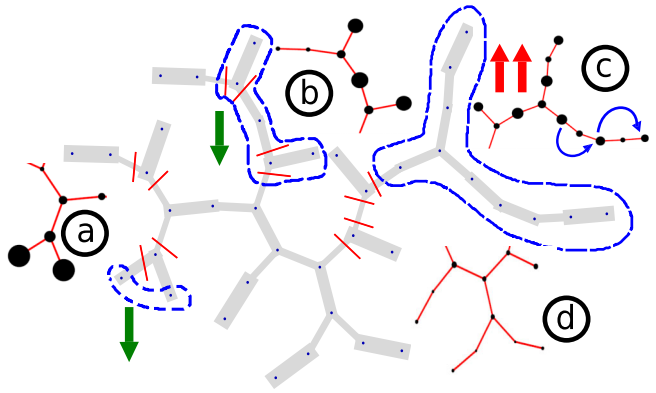

FIG. 2 (color online). Typical geometrical motifs in Cayley tree percolation clusters, as related to monomer or dimer construction. We disconnect the cluster into "spans" at the "prong" bonds, as indicated by the (red) cut lines. The (blue) dashed loops indicate regions with nonzero monomer density. The thickness of the (gray) bonds is directly proportional to $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ (with the thickest bonds having a value of ≈ -0.67). Spatial profiles associated with "dangling spins" are shown on the subclusters marked (a)–(d). The area of the black circles is proportional to ω_{ii} given by Eq. (4). (a) shows a "fork," (b) shows a site surrounded by two "prongs," (c) shows a subcluster where two monomers on the same sublattice are present forming an effective spin 1 moment. The (blue) arrows indicate the monomer is free to hop around (delocalize) within the subcluster. (d) shows a region where the spins are "inert" (largely dimerized).

"quasispin" operator $\mathbf{T}_\alpha$, where the index α labels each region on the cluster with a local spin imbalance. The $\mathbf{T}_\alpha$'s are idealized as having a spin-1/2 algebra. The actual quasispin excitation is a composite object involving multispin excitations, localized on a few sites.

Our assumption is that the quasispin quantum numbers are sufficient to label all the QD states; furthermore, we expect the action of any spin operator $\mathbf{S}_i$, when restricted to the QD states, practically reduces to a linear combination of $\mathbf{T}_\alpha$'s acting on the quasispins. Specifically, let $\hat{P}_{\mathrm{QD}}$ be the projection operator onto the QD subspace. Let $\mathbf{S}_{i,\mathrm{QD}} \equiv \hat{P}_{\mathrm{QD}} \mathbf{S}_i \hat{P}_{\mathrm{QD}}$. Then,

$$\mathbf{S}_{i,\mathrm{QD}} \cong \sum_\alpha u_i^{(\alpha)} \mathbf{T}_\alpha, \tag{2}$$

where each mode $u_i^{(\alpha)}$ has most of its weight on sites within the region α and is expected to decay rapidly outside [18].

Two operators $\hat{P}$, $\hat{Q}$ are said to be orthogonal when their Frobenius inner product $(\hat{P}, \hat{Q})_F \equiv \mathrm{Tr}(\hat{P}^\dagger \hat{Q})$ is exactly zero. In this sense, the $\mathbf{T}_\alpha$ operators are orthogonal to each other. Since each $\mathbf{T}_\alpha$ is a quasispin-1/2 operator its inner product with itself is 1/2 (for each spin component).

In light of Eq. (2), we can also construct a good approximation $\tilde{\mathbf{T}}_\alpha$ to each operator $\mathbf{T}_\alpha$ by choosing any representative site i in the region of α and normalizing the restriction of its spin operator to the QD states:

$$\tilde{\mathbf{T}}_\alpha \equiv \mathbf{S}_{i,\mathrm{QD}} / (\sqrt{2} ||\mathbf{S}_{i,\mathrm{QD}}||), \tag{3}$$

where $||\hat{O}|| \equiv (\hat{O}, \hat{O})_F^{1/2}$ is the norm of any operator $\hat{O}$. Note that the $\tilde{\mathbf{T}}_\alpha$'s are not orthogonal to each other. A procedure to construct the $\mathbf{T}_\alpha$'s from the $\tilde{\mathbf{T}}_\alpha$'s will be discussed later.

Given the proposed relationship of the bare spins to the quasispins, we discuss two related but independent measurements to recover the mode vectors $u_i^{(\alpha)}$ from numerically evaluated expectations. First, we consider the operator overlap ω_{ij} between two spins i and j on the lattice, defined to be

$$\omega_{ij} \equiv (S^+_{i,\mathrm{QD}}, S^+_{j,\mathrm{QD}})_F. \tag{4}$$

We substitute our ansatz (2) into (4) and use the operator orthogonality of the $\mathbf{T}_\alpha$'s, to get $\omega_{ij} = \sum_\alpha u_i^{(\alpha)} u_j^{(\alpha)}$. If we consider a site i to be well within a dangling region α (i.e., $u_i^{(\alpha)}$ is relatively large) then the amplitude on the remaining sites j (but far away from other dangling regions) is approximately $u_i^{(\alpha)} u_j^{(\alpha)}$. Thus, the relative amplitudes of the mode vector can be recovered by this method.

Our second measurement involves computation of the intersite spin susceptibility matrix,

$$\chi_{ij} = \int_0^\infty \langle \hat{S}_i^z(\tau) \hat{S}_j^z(0) \rangle_{GS} d\tau = \sum_n \frac{\langle 0|\hat{S}_i^z|n\rangle\langle n|\hat{S}_j^z|0\rangle}{E_n - E_0}, \tag{5}$$

where τ is imaginary time, $|0\rangle$ denotes the ground state, and E_n is the energy of an excited state $|n\rangle$ [21].

Though the sum runs over all excited states, it can be well approximated by taking only the states in the QD subspace. Then χ_{ij} can also be expressed in terms of the mode profiles $u_i^{(\alpha)}$,

$$\begin{aligned} \chi_{ij} &= \sum_{\alpha\beta} u_i^{(\alpha)} u_j^{(\beta)} X_{\alpha\beta}; \\ X_{\alpha\beta} &\equiv \sum_{n \in \mathrm{QD}} \frac{\langle 0|\mathbf{T}_\alpha^z|n\rangle\langle n|\mathbf{T}_\beta^z|0\rangle}{E_n - E_0}. \end{aligned} \tag{6}$$

Consider site $i(j)$ in dangling region α (β). From Eq. (6) it follows that $\chi_{ij} \approx u_i^{(\alpha)} u_j^{(\beta)} X_{\alpha\beta}$, where the last factor is independent of sites i, j (so long as we stay within those regions). Within this approximation, the susceptibility matrix breaks up into blocks of rank 1 from which we can immediately pull out the $u_i^{(\alpha)}$ and $u_j^{(\beta)}$ modes.

Effective Hamiltonian in the quasidegenerate subspace.—According to our ansatz (2), there is a one-to-one correspondence between the QD Hilbert space and the Hilbert space of a set of abstract quasispin operators $\mathbf{T}_\alpha$. (For simplicity, assume they all have spin 1/2.) The latter are labeled using an Ising basis $|\phi_t\rangle$, where t stands for the quantum numbers $\{t_1^z, t_2^z, \ldots, t_{n_d}^z\}$, with $t_\alpha = \pm 1/2$. We want to find the unitary matrix $\mathbf{M}$ of coefficients

expressing the QD states $|l\rangle$ (in eigenenergy basis) in terms of the quasispin basis, $|l\rangle = \sum_t M_{lt}|\phi_t\rangle$.

Using $\tilde{\mathbf{T}}_\alpha$ from (3), we define $\hat{Q}_\alpha^{\pm 1/2} \equiv ((1/2) \pm \tilde{\mathbf{T}}_\alpha^z)$, which is almost a projection operator, and let $|\tilde{\phi}_t\rangle \propto \prod_{\alpha=1}^{n_d} \hat{Q}_\alpha^{t_\alpha}|n\rangle$ where $|n\rangle$ could be any QD state (that is not annihilated by the operator prefactors) and $|\tilde{\phi}_t\rangle$ is normalized. Finally, define a matrix $\underline{\Omega}$ by $\Omega_{tt'} \equiv \langle\tilde{\phi}_t|\tilde{\phi}_{t'}\rangle$—which is almost the identity matrix—and construct the orthonormal quasispin basis of the QD states as $|\phi_t\rangle \equiv \sum_{t'}(\underline{\Omega}^{-1/2})_{tt'}|\tilde{\phi}_{t'}\rangle$. The quasispin operators $\mathbf{T}_\alpha$ are then defined so as to have the appropriate matrix elements in this basis.

Now consider the effective low-energy Hamiltonian written in terms of the many body eigenstates $|l\rangle$,

$$\mathcal{H}_{\text{eff}} \equiv \sum_{l\in\text{QD}} E_l|l\rangle\langle l| = \sum_{tt'} h_{tt'}|\phi_t\rangle\langle\phi_{t'}|, \qquad (7)$$

where E_l is the eigenenergy of QD state $|l\rangle$, and the matrix elements $h_{tt'}$ can be calculated since we know the transformation between the bases $\{|l\rangle\}$ and $\{|\phi_t\rangle\}$. Every term $|\phi_t\rangle\langle\phi_{t'}|$ can be uniquely expressed as a polynomial in the spin operators $\{T_\alpha^z\}$ and $\{T_\alpha^\pm\}$.

The effective Hamiltonian (7) then takes a new form

$$\mathcal{H}_{\text{eff}} \equiv \sum_{\mu,\nu} J_{\mu\nu}\mathbf{T}_\mu \cdot \mathbf{T}_\nu + \text{multispin terms}. \qquad (8)$$

(The two-spin terms must have this Heisenberg form due to the exact rotational symmetry retained by the QD states.)

Although the magnitude of $J_{\mu\nu}$ depends on the detailed geometry of the cluster along the path connecting dangling regions μ and ν, roughly speaking it decays exponentially with distance (using as metric the number of steps within the Bethe lattice, the so-called "chemical" distance). This is quantified by the scatter plots in Fig. 3, for an ensemble limited to clusters of equal size $N = 100$ [22] each having two dangling spin-1/2 spins ($n_d = n_{1/2} = 2$). Since each dangling region is, in general, spread out over multiple sites, we must define an "effective distance" $\bar{d}_{\mu\nu} \equiv \sum_{ij}|u_i^{(\mu)}|^2|u_j^{(\nu)}|^2 d_{ij}$ between two of them, where d_{ij} is the distance between sites i and j belonging to dangling regions μ and ν, and the amplitudes $u_i^{(\alpha)}$ for mode α are normalized.

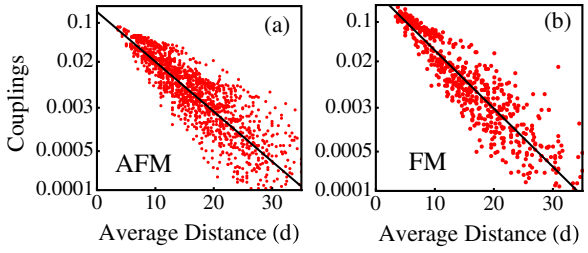

FIG. 3 (color online). Effective couplings J_{12} between two dangling spins as a function of their effective separation obtained from clusters having exactly two dangling spins. (a) dangling spins on opposite sublattices (antiferromagnetic coupling); (b) on same sublattice (ferromagnetic coupling).

Figure 3 shows that indeed $J_{\mu\nu} \approx J_0 e^{-\bar{d}_{\mu\nu}/\xi}$, where $(J_0, \xi) \approx (+0.18(3), 4.64(2))$ for a pair of dangling spins on opposite sublattices, which are always antiferromagnetically coupled, or $(-0.33(2), 4.61(3))$ for a pair on the same sublattice. In the ferromagnetic case, choosing to fit to clusters which do not form a spin 1 moment gives parameter values closer to the antiferromagnetic case.

We considered another ensemble (not plotted) of clusters with $N = 50$ having four dangling spins ($n_d = 4$) and obtained the effective Hamiltonian using the same prescription. In it, we found, the nonpair terms in (8) typically account for a weight of at most 5% (using the Frobenius norm), confirming that the effective Hamiltonian is well approximated by pairwise Heisenberg exchange (at least in the limit of dilute monomer concentration).

Conclusion.—The spin-1/2 Heisenberg antiferromagnet on Bethe lattice percolation clusters has (composite) low-energy degrees of freedom with the quantum numbers of a spin, arising wherever there is a local imbalance between the even and odd sublattices [10]. (A similar imbalance determines the low-energy spectra of regular Cayley trees [12].) Each of these emergent dangling spins is associated with a profile ($u_i^{(\alpha)}$ in the text) that plays the role of a "spinon wave function" [23]. We leave to a future publication [20] the fundamental reason why a dangling spin decouples from the rest of the cluster.

Our picture of "dangling spins" can be tested experimentally using local probes. For example, NMR at a temperature scale between the mediated interactions in (8) and the bare interactions in (1), in the presence of a field, gets a line shape mirroring the dangling-spin profile u_i, while zero-field muon spin resonance can detect the absence of an order parameter on sites away from the dangling spins.

The dangling spins interact via small, unfrustrated effective Heisenberg couplings. If one adopts the fitted exponential decay from Fig. 3 as our definition of the effective Hamiltonian, it should be possible to study clusters with thousands of sites and finally explain the scaling of the spin gap Δ_{low} with cluster size found in Refs. [10], by use of the strong disorder renormalization group method [24].

Finally, we found that spin correlations decay exponentially in balanced regions, which are dimerized, but revived on the dangling spins. This suggests locally unbalanced regions may be crucial for the propagation of long range antiferromagnetic order on percolation clusters.

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