The two-dimensional bond-diluted quantum Heisenberg model at the classical percolation threshold

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The two-dimensional antiferromagnetic $S = 1/2$ Heisenberg model with random bond dilution is studied using quantum Monte Carlo simulation at the percolation threshold (50% of the bonds removed). Finite-size scaling of the staggered structure factor averaged over the largest connected clusters of sites on $L \times L$ lattices shows that long-range order exists within the percolating fractal clusters in the thermodynamic limit. This implies that the order-disorder transition driven by bond-dilution occurs exactly at the percolation threshold and that the exponents are classical. This result should apply also to the site-diluted system.

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During the past decade, questions related to the destruction upon doping of the antiferromagnetic order in the high-$T_c$ cuprate materials have motivated extensive studies of quantum critical phenomena in two-dimensional (2D) antiferromagnets [1]. The 2D Heisenberg model on a square lattice can be driven through an order-disorder transition [2] by, e.g., introducing frustrating interactions [2] or by dimerizing the lattice [3]. It has also been believed that a non-trivial phase transition could be achieved by diluting the system, i.e., by randomly removing either sites [5–9] or bonds (nearest-neighbor interactions) [10]. The site-dilution problem is of direct relevance to the cuprates doped with nonmagnetic impurities, such as Zn or Mn substituted for Cu [11]. Early numerical work indicated that the long-range order vanishes in the Heisenberg model with nearest-neighbor interactions when a fraction $p^* \approx 0.35$ of the sites are removed [12]. Various analytical treatments have given results for $p^*$ ranging from 0.07 [13] to 0.30 [14]. These hole concentrations are below the classical percolation threshold $p_{cl} \approx 0.407$ [12], and hence the phase transition would be caused by quantum fluctuations. However, the fractal dimension and the critical exponents are the same for classical bond and site percolation [15], and our conclusions should therefore hold true also for the site-diluted system. We argue that the reason for the disagreement with the previous results by Kato et al. [15] is that they did not use sufficiently low temperatures in their simulations — extremely low temperatures are required for reaching the ground state even for the relatively small system sizes we use here.

We consider the $S = 1/2$ Heisenberg Hamiltonian on a square lattice with $N = L \times L$ sites:

$$H = \sum_{b=1}^{2N} J(b) \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)}. \quad (1)$$

The bonds $b$ connect nearest neighbor sites $i(b), j(b)$ with interaction strength $J(b) = J$ for $N$ randomly selected bonds and $J(b) = 0$ for the remaining $N$ bonds. We use an efficient finite-temperature quantum Monte Carlo method based on the “stochastic series expansion” approach [10,17] to study systems with $L = 4, 6, \ldots, 18$. In order to reach the ground state, we successively increase the inverse temperature $\beta = J/T$ until all quantities of interest have converged. We find that $\beta$ as high as $\approx 10^4$ is required for the largest lattice we have considered. Another important concern when studying random systems is the equilibration of the simulations. One would like to average over as many random configurations as possible within given computer resources. Ideally, one
would then perform only short simulations for each realization (typically, even a quite short simulation of a given configuration results in a statistical error smaller than the fluctuations between different configurations). However, there is a minimum length of a simulation set by the time needed to equilibrate it, and when carrying out short simulations it is important to have some way to verify that the correct equilibrium distribution indeed has been reached. We use the following scheme to check for both equilibration and temperature effects: For each bond configuration we carry out simulations at inverse temperatures $\beta = 2^n L$, $n = 0, 1, \ldots, n_{\text{max}}$. Starting with $n = 0$, we perform two runs for every $\beta$, each with $N_e$ updating steps for equilibration and $N_m = 2N_e$ steps for measuring physical quantities (for the definition of a “step”, see Ref. [7]). The second run is a direct continuation of the first run, so that the effective number of equilibration steps is four times that for the first run. An agreement between the results of these two runs is then a good indication that the simulation has equilibrated. For the subsequently lower temperatures (increasing $n$) we always start from the last Monte Carlo state generated at the previous temperature. The convergence of the simulations using the $\beta$-doubling procedure will be illustrated with some results below.

In the thermodynamic limit, the system at $p_{cl}$ will be spanned by infinite clusters of fractal dimension $d = 91/48$ [4]. The existence of a nontrivial (quantum) critical point is determined by the magnetic properties of these clusters. If they are long-range ordered, the critical point of the order-disorder transition driven by bond dilution will be exactly at $p_{cl} = 1/2$ as in the classical case, and the critical exponents will be the classical ones. If the fractal clusters are critical, i.e., their spin-spin correlations decay with a power-law as suggested by Kato et al. [13], the critical point is still at $p_{cl}$ but the exponents are different and non-trivial. A quantum critical point with $p^* < p_{cl}$ would imply an exponential decay of the spin-spin correlations within the fractal clusters at $p_{cl}$. In order to determine which of these scenarios apply, we have calculated the magnetization squared of the largest connected cluster of sites for a large number of random bond configurations on lattices of different linear size $L$. As $L \rightarrow \infty$ this procedure gives the ordered moment of the fractal clusters of interest. Denoting the largest cluster by $C$, the $z$-component of the staggered magnetization squared is given by

$$m^2_C = \left\langle \left( \frac{1}{N_C} \sum_{i \in C} (-1)^{x_i+y_i} S_i^z \right)^2 \right\rangle,$$

where $N_C$ is the number of spins in the cluster and the brackets indicate both the quantum mechanical expectation value and an average over bond configurations. We also consider the full staggered structure factor

$$S_x = \left\langle \frac{1}{N} \left( \sum_{i=1}^{N} (-1)^{x_i+y_i} S_i^x \right)^2 \right\rangle,$$

which involves all the spins of the lattice and was used by Kato et al. [13] to study the critical behavior of the site-diluted system. The number of random bond configurations used in the averages presented here ranges from $\approx 10^3$ for $L = 18$ to $\approx 10^4$ for $L = 4$.

In Fig. 1 we show results illustrating the equilibration scheme. The disorder-averaged $m^2_C$ is graphed versus the index $n$ (specifying the inverse temperature $\beta = 2^n L$ as described above) for $L = 18$. In order to reduce effects of fluctuations among bond realizations and more clearly show the relative effects of equilibration times and temperature, we have normalized the data to the result of the second run at the highest $\beta$ used ($n_{\text{max}} = 9$, corresponding to $\beta = 9216$) and estimated the statistical errors using the bootstrap method [18]. The number of equilibration and measurement steps were $N_e = 500$ and $N_m = 1000$. Within error bars, there are no differences between any of the equal-$\beta$ runs, and we therefore conclude that the simulations are well equilibrated. As an additional check, for $L = 16$ and smaller we have also carried out simulations using $N_e = 250$ and $N_m = 1000$ (keeping $N_m = 2N_e$). For $N_e = 250$ we do see small but statistically significant differences between the equal-$\beta$ runs, but the results of the second run are always consistent with data obtained using the longer equilibrations. Hence, we believe that our results are free of detectable
effects of insufficient equilibration. All the results to be presented below were averaged using the second of the equal-β runs only.

Fig. 1 shows that very low temperatures are needed to converge to the ground state even for a lattice of relatively modest size. Since there are no statistically significant differences between the $L = 18$ results at $\beta = 4608$ and 9216, and the asymptotic approach to the ground state should be exponential, $\beta = 9216$ should give the ground state to within error bars. In Fig. 2 we show normalized results for $S_x$ as a function of $\beta$ for all the lattices we have studied. It is clear that using a fixed $\beta = 500$ for all system sizes, as was done in Ref. [13], leads to a significant systematic error (assuming that site-diluted systems are similarly affected by temperature, which can be expected up to some factor of order 1). Fig. 2 shows that the relative deviation from the ground state grows rapidly with $L$ at fixed $\beta$ and is $\approx 3\%$ for $L = 18$ at $\beta = 500$. The largest lattice considered in Ref. [13] was $L = 48$, for which our results suggest that $\beta = 500$ could lead to an error of more than 10%. The results to be discussed below are all for $\beta = 2^9 L$.

The reason for the very high $\beta$-values needed to converge to the ground state is most likely that localized moments can form in the irregular clusters of connected spins. These moments interact with each other with a strength which decreases rapidly with increasing separation, thus leading to closely spaced energy levels. The typical level spacing should decrease faster with increasing $L$ than the $1/L$ behavior suggested in Ref. [3]. The temperature effects should be the largest exactly at the percolation threshold and for all hole concentrations they lead to an underestimation of the ordered moment. Hence, the result that there is a substantial order in the system close to the percolation threshold [13] should remain valid despite such effects.

In order to definitely determine whether indeed $p^* = p_{c1}$ and whether or not the exponents are the classical ones, we here study the lattice-size dependence of the cluster order parameter squared; Eq. (2). As a finite-size scaling ansatz, we use a simple generalization of the known scaling law for the sublattice magnetization $m$ for the pure 2D Heisenberg model. In that case the leading size-correction to $m^2$ is $\sim 1/N^{1/2}$ [12], which can be seen clearly in numerical data [20]. Since the average number of spins in the fractal clusters of the diluted system depends asymptotically on $L = N^{1/2}$ according to $\langle N_C \rangle \sim L^d$, with $d$ the fractal dimension quoted above, we here assume a leading size correction $\sim 1/L^{d/2}$. Fig. 3 shows our data for $m^2_C$ graphed versus this variable. The results appear to be consistent with the ansatz, although in order to fit all the data points we have to use a polynomial cubic in $1/L^{d/2}$ (a cubic polynomial is needed also to fit data for the pure 2D Heisenberg model, but the corrections to the linear behavior are much smaller [20]). This fit has a $\chi^2$ per degree of freedom of $\approx 0.6$ and gives the full staggered magnetization $M_\nu = \sqrt{3m^2_C} \approx 0.09$ for the infinite fractal clusters (the factor 3 accounts for rotational averaging). Hence, the order on the $d$-dimensional fractal lattice is as high as $\approx 30\%$ of the 2D staggered moment [20].

Finally, we discuss results for the staggered structure factor of the full lattice; Eq. (3). In Fig. 4 we graph $\ln \langle S_x \rangle$ versus $\ln (L)$, which should show an asymptotic linear scaling behavior. There is a clear upward curvature
as the lattice size increases, and it is clear that we are still far from the scaling regime. A curvature is also seen in the data presented by Kato et al. for small systems [13], but for larger sizes a linear behavior was discerned. As we have discussed above, the structure factor calculated for large lattices in Ref. [13] was likely substantially underestimated due to temperature effects, and the apparent non-classical scaling behavior is then an artifact. Since the results in Fig. 4 show that there is long-range order in the fractal clusters, the growth of \( S_\pi \) must asymptotically be given by classical percolation theory, i.e., \( S_\pi \sim L^{d-2} \), where \( 2d - 2 = 43/24 \). The very large corrections to scaling evident in Fig. 4 can be understood as resulting from a significant reduction with increasing \( L \) of the staggered structure factor per site of the fractal clusters (\( m_C^2 \)), as seen in Fig. 4. Classically, \( m_C^2 \) is independent of system size and the scaling of \( S_\pi \) is therefore determined solely by the increase in size of the clusters as \( L \) increases. In the quantum case, the size dependence of \( S_\pi \) is dominated by this geometric effect only for system sizes sufficiently large for the relative size-correction to \( m_C^2 \) to be small. For our largest lattice, the relative size-correction is still more than a factor four. Considering the extremely low temperatures required to study the ground state of large lattices, it will be very difficult to numerically observe the asymptotic classical scaling regime for \( S = 1/2 \).

In summary, we have presented numerical results showing that the fractal \( S = 1/2 \) Heisenberg clusters at the classical bond-percolation density have long-range antiferromagnetic order. This implies that the order-disorder transition driven by bond-dilution occurs exactly at the percolation density and that the critical exponents are classical. This should hold true for any spin \( S \), and since classical bond and site percolation are equivalent in terms of the fractal dimension and the critical exponents [13], our conclusions should apply also to the site-diluted model. The quantum mechanical corrections to the asymptotic scaling behavior are very large for lattice sizes that can be studied with today’s computers, making direct observation of the critical behavior difficult. We have also discussed temperature effects and shown that extremely low temperatures are needed to study the ground state, likely due to the presence of weakly interacting localized moments.

It would be interesting to study a diluted system including frustration. If the clean system is already close to a quantum critical point, non-magnetic impurities may be able to drive it into a quantum disordered phase. The fact that Zn or Mn doping of the cuprates destroys the long-range order well before the classical percolation threshold [11] clearly indicates that these materials cannot be described by a randomly diluted Heisenberg model with nearest-neighbor interactions only.

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