Quantum Phase Transition of
Two-Dimensional Diluted Heisenberg Antiferromagnet

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Quantum phase transition of site-diluted and bond-diluted Heisenberg antiferromagnets on square lattices is studied. By using the novel continuous-time loop algorithm, we perform quantum Monte Carlo simulations on quite larger lattices at extremely lower temperatures than the previous numerical studies. It is found that the antiferromagnetic long-range order at $T = 0$ persists so long as a cluster of magnetic sites percolates, that is, the critical concentration is equal to the classical percolation threshold, in both of the site-diluted and bond-diluted cases. Furthermore, we find that some critical exponents, such as the magnetization exponent β, are non-classical and strongly depend on the spin size S. On the other hand, we show that the correlation-length exponent ν is universal and is equal to the classical value ($\nu = 4/3$).

§1.   Introduction

Recently, by the development of cluster algorithms, such as the loop algorithm,[1]-[7] the quantum Monte Carlo (QMC) techniques[8] have been improved greatly. Together with the enhancement of the computer performance itself, it enables us to perform large-scale and highly precise simulations on spin systems with strong quantum fluctuations, which sometimes leads us to completely new physical findings not only quantitatively but also qualitatively. In this paper, we report one of such results of the QMC simulations on the randomly-diluted Heisenberg antiferromagnet (HAF) on a square lattice.

In the classical limit, i.e., $S = \infty$, the diluted HAF at zero temperature is equivalent to the percolation model.[9] For the site percolation on a square lattice, the percolation threshold is obtained as $p_{cl} = 0.5927460(5)$ by the most recent simulation.[10] On the other hand, for the bond percolation, p_{cl} is shown to be $1/2$ analytically.[9] For $S < \infty$, the classical percolation threshold p_{cl} still gives an *exact* lower bound for the critical concentration of the ground-state antiferromagnetic long-range order. One of the most important, but unsettled, questions is whether the existence of quantum spin fluctuations makes the critical concentration deviate form p_{cl}, or not.

In the previous studies, it is suggested that the critical concentration of the quantum system is larger than the classical percolation threshold for the site-diluted model [11)-13)] and also for the bond-diluted one. [14)] In this paper, by using the continuous-time loop algorithm, [1)-7)] we perform QMC simulation on larger systems ($L \times L = 48 \times 48$) at quite lower temperatures ($T = 0.0005$) than the previous works. We study the site-diluted and the bond-diluted HAF's, and show that the critical concentration (we refer to it as p^*) is equal to the classical percolation threshold $p_{\rm cl}$ in both cases. We also discuss the critical property of the present quantum phase transition at $p = p_{\rm cl}$ in detail.

§2.   Models

We consider the site-diluted and the bond-diluted HAF's, whose Hamiltonians are defined as

$$\mathcal{H} = \sum_{\langle i,j \rangle} \epsilon_i \, \epsilon_j \, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{2·1}$$

and

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{i,j} \, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \,, \tag{2·2}$$

respectively. The quenched dilution factors $\{\epsilon_i\}$ (or $\{J_{i,j}\}$) take 1 or 0 independently with probability p and $1 - p$, respectively, where p denotes the concentration of magnetic sites (or bonds). We consider $L \times L$ square lattices with periodic boundary conditions in both cases.

It is well known that traditional world-line Monte Carlo methods, [8)] based on local updates of world line configuration, suffer from strong correlation between successive configurations at low temperatures. This drawback is solved almost completely by the loop algorithm. [1)-3),5)] It often reduces the auto-correlation time by orders of magnitude. In the present simulation, we use the continuous-time loop algorithm [4)] extended to general-S cases, [6),7)] which works directly in the Trotter limit. Another important feature of the present algorithm is its ergodicity; the winding number of world lines around vacant sites can change and the ground-canonical ensemble also can be simulated.

We mainly concentrate on the static structure factor at $T = 0$,

$$S_{\rm s}(L, p) = \lim_{T \to 0} \frac{1}{L^d} \sum_{i,j} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} \langle S_i^z S_j^z \rangle \tag{2·3}$$

at momentum $\vec{k} = (\pi, \pi)$. Here, d is the spatial dimension ($d = 2$). The bracket in Eq. (2·3) denotes both of the thermal average and the average over samples. In the present simulation, we use an improved estimator, which reduces the variance of data greatly. In order to obtain the zero-temperature value, we perform QMC simulations at low enough temperatures so that $S_{\rm s}$ exhibits no temperature dependence besides statistical errors. The lowest temperature used in the present simulation is $T = 0.0005$. For each sample, 10^4 Monte Carlo steps (MCS) are spent for measurement

after 10^3 MCS for thermalization. At each parameter set (L, T, p), physical quantities are averaged over $10^2 - 10^4$ samples depending on L, T, and p.

§3. Results

The staggered magnetization $M_s(p)$ is calculated as

$$M_s^2(p) = \lim_{L \to \infty} \frac{3S_s(L, p)}{L^d} . \tag{3·1}$$

As is clearly seen in Fig. 1, $M_s(p)$ remains finite even at $p = 0.625$ for the site-diluted cases with $S = 1/2$ and 1. [15] Therefore, the possibility that $p^* = 0.655$ or 0.695, which have been suggested by the previous QMC simulation [11] and the analytic approach based on mapping to the non-linear σ model, [13] respectively, is excluded definitely.

In Fig. 2, we show the system size dependence of $S_s(L, p)$ just at the classical percolation threshold for the site-diluted cases with $S = 1/2$ and 1 and also for the $S = 1/2$ bond-diluted case. We observe no tendency of saturation for large L in all the cases, which strongly supports that $p^* = p_{cl}$. Furthermore, the data for larger systems ($L \geq 20$) exhibits a clear power-law behavior

$$S_s(L, p_{cl}) \sim L^\Psi . \tag{3·2}$$

For the site-diluted cases with $S = 1/2$ and 1, the value of exponent Ψ is estimated as $1.17(6)$ and $1.57(3)$, respectively, by least-squares fitting for the data with $L \geq 24$. [15] It should be emphasized that Ψ's for $S = 1/2$ and 1 differ definitely with each other, and furthermore both of them are significantly smaller than the classical value ($\Psi = 43/24 = 1.7917$). [9] For the bond-diluted case, one can also find that the static structure factor tends to diverge. However, we observe larger corrections to scaling
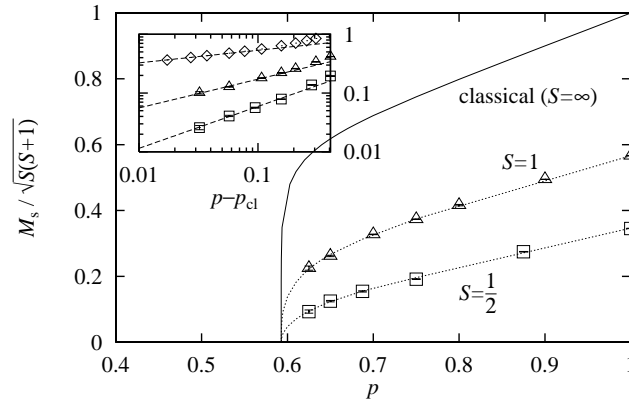

Fig. 1. Concentration dependence of the staggered magnetization of the site-diluted models with $S = 1/2$, 1, and ∞. The dotted lines are guide to eye. In the inset, we show the double-logarithmic plot of the staggered magnetization against $(p - p_{cl})$. The dashed lines are obtained by least-squares fitting for $p \leq 0.70$.
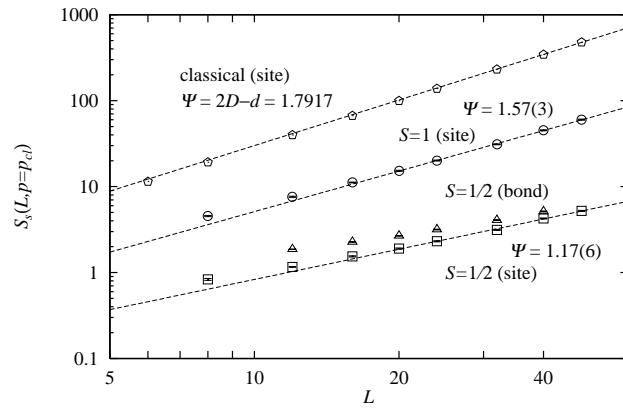
Fig. 2. System-size dependence of the static structure factor at the percolation threshold ($p = p_{\rm cl}$). The dashed lines are obtained by least-squares fitting for $L \geq 24$.
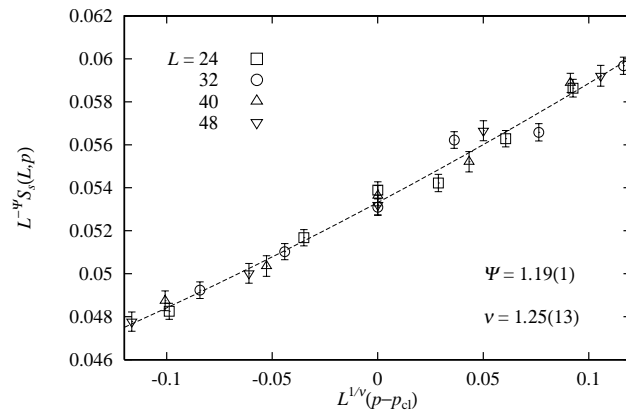

Fig. 3. Scaling plot of the static structure factor of the $S = 1/2$ site-diluted HAF. The critical concentration is assumed to be equal to the percolation threshold.

in comparison with the site-diluted case (Fig. 2). We obtained $\Psi = 1.05$ from the data with $L = 32$ and 40, which is slightly smaller than that in the site-diluted case.

Next, we consider the correlation-length exponent ν. We perform finite-size scaling analysis for the static structure factor of the $S = 1/2$ site-diluted model with $0.585 \leq p \leq 0.605$ by assuming $p^* = p_{\rm cl}$. As seen in Fig. 3, the data with $L \geq 24$ are scaled fairly well with $\Psi = 1.19(1)$ and $\nu = 1.25(13)$. The value of Ψ is consistent with that obtained by the scaling analysis at $p = p_{\rm cl}$ (Fig. 2). Note that on the other hand, the value of ν coincides with the classical value ($\nu = 4/3$) [9] within the error bar.

§4. Summary and discussion

In the present paper, we have investigated the ground-state phase transition of the diluted HAF. Contrary to the previous works, [11]-[14] our present QMC study has

shown that the critical concentration is equal to the classical percolation threshold even in the $S = 1/2$ case. On the other hand, it is found that the transition is non-universal; the critical exponents depend on the spin size S. This means that not only the fractal nature of the lattice geometry at $p = p_{cl}$, but also the strength of the quantum fluctuation, controlled by the spin size S, are relevant in the present quantum phase transition. The criticality at $p = p_{cl}$ might be characterized by an S-dependent exponent α, which is defined in terms of the staggered spin correlation function between two sites on a fractal cluster as

$$C(i, j) \sim r_{i,j}^{-\alpha} \quad \text{for } r_{i,j} \gg 1. \tag{4.1}$$

In the classical case, $C(i, j)$ takes a constant value, and therefore $\alpha = 0$. Together with the cluster-size distribution at $p = p_{cl}$, predicted by the percolation theory, [9] we obtain a scaling relation between the S-dependent exponents Ψ and α:

$$\Psi = 2D - d - \alpha, \tag{4.2}$$

where D is the fractal dimension ($D = 91/48$).

On the other hand, the critical exponent ν has been found to be unmodified from the classical value ($\nu = 4/3$) within the present numerical uncertainty (Fig. 3). We can also obtain the exponent β from the staggered magnetization at $p > p_{cl}$ as $\beta = 0.46(3)$ and $0.32(3)$ for the $S = 1/2$ and 1 site-diluted model, respectively (Fig. 1). By using a scaling relation [15]

$$2\beta = -(2D - 2d - \alpha)\nu = (d - \Psi)\nu, \tag{4.3}$$

we obtain $\nu = 1.2(1)$ and $1.5(2)$, respectively. These values are also consistent with $\nu = 4/3$. This implies that there is no macroscopic length scale other than the geometrical length scale, [15] which is defined as the average size of finite clusters in the percolation theory. [9]

Quite recently, the $S = 1/2$ bond-diluted model is reexamined by using the stochastic series expansion. [17] Contrary to the previous study, [14] it is concluded that the critical concentration is equal to the percolation threshold, which is consistent with the present study. However, it is suggested furthermore that the critical exponents are unmodified from the classical values. The reason of this disagreement is now being examined, but we believe that it might be due to smallness of the system size, ($L \leq 18$) or improper scaling assumption made in Ref. 17).

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