Bond-Dilution Effects on Two-Dimensional Spin-Gapped Heisenberg Antiferromagnets

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Abstract
Bond-dilution effects on spin-1/2 spin-gapped Heisenberg antiferromagnets of coupled alternating chains on a square lattice are investigated by means of the quantum Monte Carlo method. It is found that, in contrast with the site-diluted system having an infinitesimal critical concentration, the bond-diluted system has a finite critical concentration of diluted bonds, $x_c$, above which the system is in an antiferromagnetic (AF) long-range ordered phase. In the disordered phase below $x_c$, plausibly in the concentration region significantly less than $x_c$, the system has a spin gap due to singlet pairs of induced magnetic moments reformed by the AF interactions through the two-dimensional shortest paths.

1. Introduction
Impurity effects on quantum Heisenberg antiferromagnets with a spin gap due to the topological structure of the system have attracted much interest in relation to the impurity-induced antiferromagnetic (AF) long-range order (LRO) observed experimentally \cite{1,2,3,4}. There are two types of disorders, i.e., site dilution and bond dilution. Extensive theoretical and numerical works have investigated properties of diluted Heisenberg antiferromagnets in the one-dimensional (1D) \cite{5,6} and two-dimensional (2D) systems. In the latter, however, the interchain interactions have been treated by the mean-field-type approximations \cite{7}, so that the difference of these two types of disorders cannot be naturally introduced. In the present paper we have investigated bond-dilution effects on the spin-1/2 spin-gapped AF Heisenberg system by treating the interchain interactions on the equal footing as the intrachain interactions by means of the quantum Monte Carlo (QMC) method. The result obtained clearly reveals the different aspects between magnetic properties of the bond- and site-diluted systems.

The site-dilution effects have been already extensively investigated \cite{8,9,10}. If spins are randomly removed from the lattice, magnetic moments are induced at sites neighboring the removed sites. We have called the domain of induced magnetic moments the ‘effective spin’. They situate centered at sites next to each removed spin, and their extent is given by the correlation lengths, $\xi_{x,y}^p$, of the non-diluted system. The effective exchange coupling between two effective spins centered at sites $m$ and $n$ is given by $\tilde{J}_{mn} \propto (-1)^{|r_m-r_n+1|}\exp[-l/(\xi_{x,y}^p)^{1/2}]$, where $l = |r_m-r_n|$ is the distance between the effective spins \cite{11,12}. There exist strong correlations...
between the effective spins retaining the staggeredness with respect to the original lattice [10]. Therefore, the 2D site-diluted system has an AF LRO induced with an infinitesimal concentration of dilution at zero temperature.

On the other hand, if a certain bond is removed from the lattice, the effective spins, peaks of which are located at both ends of the diluted bond, are induced. In this case, besides the same interaction $J_{mn}$ between spins next to different removed bonds as in the site-diluted case, there exist AF interactions $J_{AF}$ between two spins at both ends of a removed strong bond through the 2D shortest paths. The latter is estimated of the order of $\frac{1}{\xi}$, where $\xi$ is the average for dilution is taken over $10^3 \sim 10^4$ Monte Carlo steps (MCS) are spent for measurement after $500 \sim 10^3$ MCS for thermalization. Sample average for dilution is taken over $10 \sim 10^3$ samples.

2. Model and method

We investigate the bond-diluted quantum AF Heisenberg model of coupled alternating chains on a square lattice described by the Hamiltonian

$$H = \sum_{i,j} \epsilon_{(2i+1,j)} S_{2i,j} \cdot S_{2i+1,j} + \alpha \sum_{i,j} \epsilon_{(2i+1,j)} S_{2i+1,j} \cdot S_{2i+2,j} + J' \sum_{i,j} \epsilon_{(i,j+1)} S_{i,j} \cdot S_{i,j+1} ,$$

where $1$ and $\alpha (>0)$ are the AF intrachain alternating coupling constants, $J' (>0)$ the AF interchain coupling constant, and $S_{i,j}$ the quantum spin operator with $S = 1/2$ at site $(i,j)$. Randomly quenched bond occupation factors $\{\epsilon_{(i,j)}\}$ independently take either $1$ or $0$ with probability $1-x$ and $x$, respectively, where $x$ is the concentration of diluted bonds. The pure system described by Eq. (1) with $\epsilon_{(i,j)} = 1$ for all bonds is in a spin-gapped or an AF LRO phase depending on strengths of $\alpha$ and $J'$ at zero temperature [13].

In the $\alpha = 0.5$ system which we examine in the present work there exists the spin-gapped phase below $J'_c \simeq 0.55$.

The QMC simulations with the continuous-imaginary-time loop algorithm [14,15,16] are carried out on $L \times L$ square lattices with the periodic boundary conditions. For each sample with a bond-diluted configuration, $10^3 \sim 10^4$ Monte Carlo steps (MCS) are spent for measurement after $500 \sim 10^3$ MCS for thermalization. Sample average for dilution is taken over $10 \sim 10^3$ samples.

3. Numerical results

The $x$ dependences of the staggered magnetization $M_s$ in the bond- and site-diluted [10] systems with $\alpha = J' = 0.5$ are shown in Fig. 1. If the pure system with the spin-gapped state is diluted, the AF LRO is induced at a certain concentration in both site- and bond-diluted cases. However, whereas the site-diluted system is driven into the AF LRO phase by an infinitesimal concentration, in the bond-diluted system there exists a critical concentration of $x_c \simeq 0.05$ even for $\alpha = J' = 0.5$, which is the system near the critical point $J'_c \simeq 0.55$ for $\alpha = 0.5$ and $x = 0$. As the value of $J'$ becomes smaller, the region of the disordered phase,
whose strengths are 1, \( \alpha \), and \( J' \), respectively. If a weaker bond with \( \alpha \) or \( J' \) is removed, the singlet pairs on the strong bonds are not disturbed at all and so magnetic moments are not induced. However, if a strong bond is removed, magnetic moments are induced at both ends of the diluted bond. In Fig. 2(a) the real-space distribution of the local static staggered structure factor defined by \( S(i) \equiv \sum_j (-1)^{|r_i-r_j|} \langle S_i^z S_j^z \rangle \) is shown for \( \alpha = 0.5 \) and \( J' = 0.3 \) on a 64 \( \times \) 64 lattice from which 15 diluted strong bonds are removed. We can clearly see that magnetic moments are always induced at both ends of a diluted bond reform a singlet pair due to the effective interaction \( J_{AF} \) through the 2D shortest paths. We note here that since induced magnetic moments are located at sites of the different sublattices, the interaction is always AF. As \( J'^2 \) is increased, \( \Delta \) deviates from the proportionality to \( J'^2 \). This indicates that the localized singlet picture does not hold well for larger values of \( J' \).

In the inset of Fig. 4 the \( T \) dependence of the effective Curie constant \( \chi(x)T \) for \( \alpha = 0.5 \) and \( J' = 0.3 \) is shown at \( x = 0.04, 0.02, 0.01, \) and 0 from top. The uniform susceptibility \( \chi(0) \) exponentially decreases at low temperatures due to the spin gap with the value of 0.31415(2). In the main frame of Fig. 4, the differences \( (\chi(x) - \chi(0))T \) are shown.
The plateau with the Curie constant proportional to \(x\) is clearly seen in these plots and \((\chi(x) - \chi(0))T\) falls off exponentially at lower temperature than \(J'^2 = 0.09\). This confirms again the existence of the spin gap due to \(J_{AF}\) at relatively small \(x\).

4. Summary and discussion

When bonds are randomly removed in the spin-gapped phase, the AF effective interaction \(J_{AF}\) between two spins at both ends of a removed strong bond is induced in addition to the effective interaction \(\tilde{J}_{mn}\) between spins on ends of different removed bonds. Therefore, in such a low-concentration region that the strength of \(J_{AF}\) is larger than \(|\tilde{J}_{mn}|\) there exists the spin-gapped phase dominated by \(J_{AF}\).

The ground state of the diluted dimerized 1D system with \(J' = 0\) and \(x > 0\) is in the quantum Griffiths phase, which is characterized by the finite correlation length and the gapless excitation. In the present 2D system with \(J' > 0\) our numerical results strongly suggest a gapless phase but without AF LRO just below \(x_c\). The problem will be discussed elsewhere.

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