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Quantum Monte Carlo Simulation of S=1/2 Heisenberg model with Four Spin Interaction

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Abstract. The spin $S = 1/2$ Heisenberg model with four-spin interaction on the square lattice is studied by using quantum Monte Carlo method. When the four-spin interaction is dominant, the system has a VBS ground state. In this case, we find a finite-temperature second-order phase transition to the VBS state. The universality class of the transition is investigated. We estimate the critical exponents ν and η from the finite size scaling analysis and find $\nu = 0.68(1)$ and $\eta = 0.55(2)$.

1. Introduction

Recently, Senthil *et al.* proposed [1, 2] a new theory of a quantum critical point named *deconfined critical point* (DCP). According to the theory, a second-order phase transition from the Néel state to a valence-bond-solid (VBS) state is possible at the DCP. In the VBS state, each spin forms a singlet dimer with one of their neighbors, breaking the lattice rotational symmetry. In contrast to the DCP theory, a direct second-order transition from the Néel state to the VBS state is forbidden in the conventional Landau-Ginzburg-Wilson framework. The proposal of the DCP stimulated many attempts to find a spin model that has a second-order transition between the Néel state and the VBS state.

Sandvik proposed[3] an $S = 1/2$ Heisenberg model with four-spin interaction on the square lattice, which is described by the Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - Q \sum_{\langle p \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4})(\boldsymbol{S}_k \cdot \boldsymbol{S}_l - \frac{1}{4}), \tag{1}$$

where $J, Q > 0$ and summation over $\langle i, j \rangle$ and $\langle p \rangle$ are taken for all nearest-neighbor pairs and all plaquettes of the square lattice, respectively. Sites i,j,k and l in the second term of the Hamiltonian (1) are sites on the corners of the plaquette p. For each plaquette, the pairs of the sites (i, j) and (k, l) are taken twice in such a way that the nearest-neighbor bond connecting sites i and j is parallel to that connecting k and l. This model was calculated using projector Monte Carlo method[4] and it was found[3] that the ground state is the VBS state when J/Q=0 and there is a second-order quantum phase transition to the Néel state at $J/Q = (J/Q)_c = 0.04$. Furthermore, these results were confirmed by Melko and Kaul[5]. However, there is also a claim [6] that the transition is a weak first-order transition. The quantum criticality of this model is an unanswered problem at present.

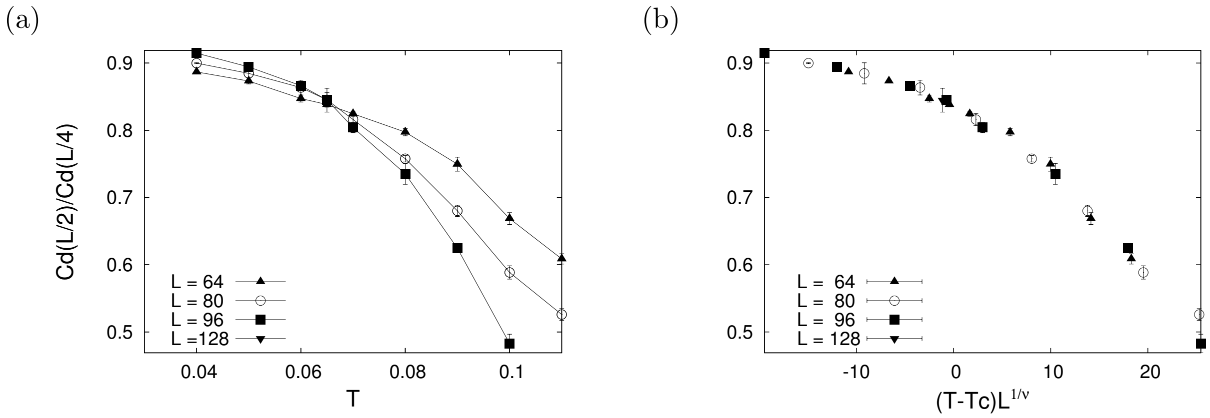

Figure 1. (a) Temperature dependence of the correlation ratio with various system size L. There is a second-order phase transition at T = 0.065. (b) Scaling plot of the correlation ratio using $T_{\mathrm{c}} = 0.065$ and $\nu = 0.68$.

In addition to the critical nature of the transition point, the nature of the VBS state of the model is also unclear[7, 3, 6]. In the theory of the DCP, the VBS state is a state where the lattice Z_4 symmetry is broken and fourfold degenerate[2]. However, histograms of the dimer order parameters that distinguish the degenerated states did not show any sign of the Z_4 symmetry breaking in the VBS state[7, 3, 6].

In the present paper, we focus on the VBS state of the model described by the Hamiltonian (1) and study the finite-temperature phase transition to the VBS state when $J/Q = 0$ using quantum Monte Carlo method. We investigate the universality class of the transition to check if the Z_4 nature of the model manifests itself in the VBS state.

2. Finite Temperature Phase Transition to the VBS State

Since the lattice symmetry is broken in the VBS state, there can be a finite temperature phase transition in the two dimensional system because of the discreteness of the symmetry. Especially, if the system breaks the Z_4 symmetry, the transition belongs to the universality class of the isotropic Ashkin-Teller (AT) model[8]. It is well-known that the exponent η of the AT model has a unique value of $\eta = \eta_{\mathrm{Z}_4} = 1/4$, while the criticality of the AT model is not universal[9]. We investigate the finite temperature phase transition to the VBS state and check if it belongs to the universality class of the transition where the Z_4 symmetry breaks.

To estimate the transition temperature, we compute the correlation of the dimerization order parameter $C_{\mathrm{d}}(r)$ defined as

$$C_{\mathrm{d}}(r) = \frac{1}{N}\langle \sum_i S_i^{\mathrm{z}} S_{i+\boldsymbol{e}_{\mathrm{x}}}^{\mathrm{z}} S_{i+r\boldsymbol{e}_{\mathrm{x}}}^{\mathrm{z}} S_{i+(r+1)\boldsymbol{e}_{\mathrm{x}}}^{\mathrm{z}} \rangle - \frac{1}{N^2}\langle \sum_i S_i^{\mathrm{z}} S_{i+\boldsymbol{e}_{\mathrm{x}}}^{\mathrm{z}} \rangle^2, \quad (2)$$

where $\boldsymbol{e}_{\mathrm{x}}$ is the lattice unit vector in the x direction. Near the critical point , the correlation scales as

$$C_{\mathrm{d}}(r) \sim r^{d-2-\eta} f(L/\xi) \sim r^{d-2-\eta} f(L(T-T_{\mathrm{c}})^{\nu}), \quad (3)$$

where ξ is the correlation length and ν and η are critical exponents. If we plot the correlation ratio[10] $C_{\mathrm{d}}(L/2)/C_{\mathrm{d}}(L/4)$ as a function of temperature with various system size L, the data cross at the critical temperature T_{c}. Figure 1(a) shows the temperature dependence of the correlation ratio. The crossing point at $T = 0.065$ in the figure indicates that there is a second-order phase transition at the point. We perform a finite-size scaling of the correlation ratio using the hypothesis Eq. (3) and obtain $\nu = 0.68(1)$ (See Fig. 1(b)).

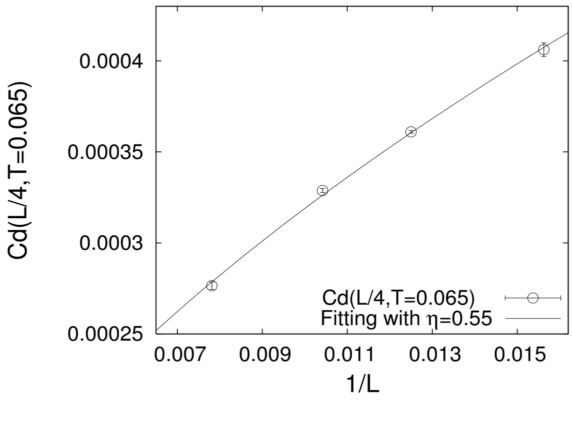

Figure 2. System size dependence of the $C_{\rm d}(L/4, T = 0.065)$. The data is fitted to the form $C_{\rm d} \sim L^{-\eta}$ and we obtain $\eta = 0.55(2)$.

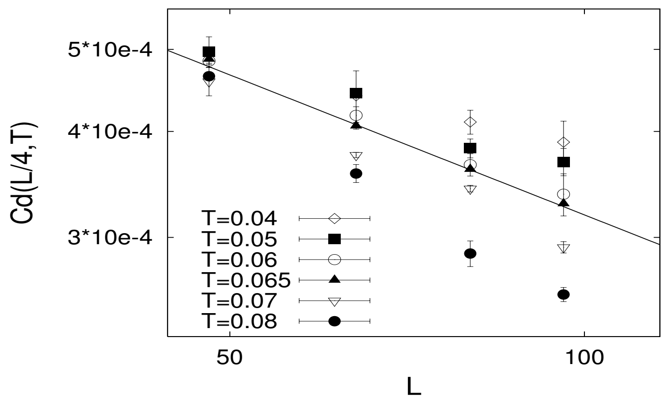

Figure 3. Logarithmic plot of the system size dependence of the $C_{\rm d}(L/4)$ with various temperatures. The line in the figure is a fitting plot with $C_{\rm d} \sim L^{-0.55}$. The data above (below) $T = 0.065$ deviate upward (downward) from the line.

We can estimate the exponent η from the scaling form of the dimer correlation at the critical point $C_{\rm d}(L, T = T_{\rm c}) \sim L^{-\eta}$. The estimated value of is $\eta = 0.55(2)$ (See Fig. 2). To check the validity of the above estimations of $T_{\rm c}$ and η, we show a logarithmic plot of the $C_{\rm d}(L/4)$ vs. L with various temperatures around $T = 0.065$ in Fig. 3. The line of the figure is a fitting using the scaling form $C_{\rm d} \sim L^{-\eta}$ with $\eta = 0.55$. The data of $T = 0.065$ is on the straight line while the data of other temperatures deviate from the line.

3. Conclusions and Discussions

As we have seen above, the estimated value of the exponent $\eta \sim 1/2 \neq \eta_{Z_4}$. This is not surprising at the first glance because we have not observed any Z_4 character in the order-parameter distribution function. However, since the distribution looks U(1) symmetric[3, 6], we could at least observe a transient, most likely the KT-type, behavior. It is puzzling that we do not observe any KT-like behavior, either. This may indicate that transition may belong a new universality class.

To conclude, we have simulated the Heisenberg model with four-spin interaction and observed the finite temperature phase transition to the VBS state when the four-spin interaction is dominant. While the Z_4 symmetry breaking was expected at the transition point, the estimated value of the exponent η was different from that of the universality class of the transition where Z_4 symmetry breaks.

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