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 $\nu$ and $\eta$ 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

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

(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.
There is a second-order phase transition at $T = 0.065$. 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)).

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 $\eta$ of the AT model has a unique value of $\eta = \eta_{Z_4} = 1/4$, 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 $C_d(r)$ defined as

$$C_d(r) = \frac{1}{N} \left( \sum_i S_i^x S_{i+x}^x, e_x S_i^z S_{i+1}^z e_x \right) - \frac{1}{N^2} \left( \sum_i S_i^x S_i^z e_x \right)^2,$$

where $e_x$ is the lattice unit vector in the $x$ direction. Near the critical point, the correlation scales as

$$C_d(r) \sim r^{d-2-\eta} f(L/r) \sim r^{d-2-\eta} f(L(T_c)^\nu),$$

where $\xi$ is the correlation length and $\nu$ and $\eta$ are critical exponents. If we plot the correlation ratio[10] $C_d(L/2)/C_d(L/4)$ 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 $C_d(L/4, T = 0.065)$. The data is fitted to the form $C_d \sim L^{-\eta}$ and we obtain $\eta = 0.55(2)$.

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

We can estimate the exponent $\eta$ from the scaling form of the dimer correlation at the critical point $C_d(L, T = T_c) \sim L^{-\eta}$. The estimated value of is $\eta = 0.55(2)$ (See Fig. 2). To check the validity of the above estimations of $T_c$ and $\eta$, we show a logarithmic plot of the $C_d(L/4)$ vs. $L$ with various temperatures around $T = 0.065$ in Fig. 3. The line of the figure is a fitting using the scaling form $C_d \sim L^{-0.55}$ 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 $\eta$ was different from that of the universality class of the transition where $Z_4$ symmetry breaks.

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