Variational study of the quantum phase transition in the bilayer Heisenberg model with bosonic RVB wavefunction

Haijun Liao and Tao Li

Department of Physics, Renmin University of China, Beijing 100872, People’s Republic of China

Received 19 July 2011, in final form 5 October 2011
Published 10 November 2011
Online at stacks.iop.org/JPhysCM/23/475602

Abstract

We study the ground state phase diagram of the bilayer Heisenberg model on a square lattice with a bosonic resonating valence bond (RVB) wavefunction. The wavefunction has the form of a Gutzwiller projected Schwinger boson mean-field ground state and involves two variational parameters. We find the wavefunction provides an accurate description of the system on both sides of the quantum phase transition. In particular, through the analysis of the spin structure factor, ground state fidelity susceptibility and the Binder moment ratio $Q_2$, a continuous transition from the antiferromagnetic ordered state to the quantum disordered state is found at the critical coupling of $\alpha_c = J_\perp/J_\parallel \approx 2.62$, in good agreement with the result of quantum Monte Carlo simulation. The critical exponent estimated from the finite size scaling analysis ($1/\nu \approx 1.4$) is consistent with that of the classical 3D Heisenberg universality class.

(Some figures may appear in colour only in the online journal)

1. Introduction

The study of quantum phase transitions is a central issue in modern condensed matter physics. It is widely believed that the Ginzburg–Landau–Wilson theory for classical phase transitions may fail to describe the quantum phase transition as a result of the quantum interference effect between classical paths (the Berry phase effect). Recently, the concepts of quantum order and de-confined quantum criticality have been put forward theoretically. On the experimental side, the study of quantum phase transitions plays an important role in areas ranging from high-$T_c$ cuprates, heavy fermion systems, to the cold-atom systems [1].

The bilayer Heisenberg model (BHM) on a square lattice is a standard model for the study of quantum phase transitions. With the increase of the interlayer coupling ($J_\perp$) over the intralayer coupling ($J_\parallel$), the ground state of the system evolves from a state with antiferromagnetic long range order to a quantum disordered state through a continuous phase transition. Much theoretical and numerical effort has been devoted to the study of this quantum phase transition.

On the theoretical side, perturbative calculations starting from both the ordered side (spin wave expansion) [2] and the disordered side (bond operator expansion) [3] have been applied to the system. However, due to the biased nature of perturbative methods, none of them can give an accurate description of the system in the near-vicinity of the quantum phase transition. The problem is also treated with the Schwinger boson mean-field theory [4, 5]. Although the theory does predict a phase transition between the antiferromagnetic ordered state and the quantum disordered state, the nature of the transition is incorrect. The mean-field theory predicts a discontinues dimerization transition around $J_\perp/J_\parallel = 4.62$ into a state composed of independent interlayer dimers, while in the real system the intralayer correlation is nonzero for any finite $J_\perp/J_\parallel$.

On the numerical side, the model is thoroughly studied by a variety of methods including the high temperature series expansion [6] and the quantum Monte Carlo simulation (stochastic series expansion) [7, 8]. These numerical works confirm the existence of the quantum critical point around $\alpha = J_\perp/J_\parallel \approx 2.52$. The critical exponent is found to be consistent with that of the classical 3D Heisenberg universality class, indicating the irrelevance of the Berry phase effect in this phase transition.
As the quantum phase transition occurs at zero temperature, it is natural to find a description of it in terms of an explicit ground state wavefunction. The variational approach to quantum phase transitions has the virtue that it focuses directly on the zero-temperature behavior of the system and provides much more detailed information on the quantum critical behavior. In this regard, a resonating valence bond (RVB)-type variational wavefunction [11, 12] had been applied to the study of the quantum phase transition in the BHM. The wavefunction is derived from the Gutzwiller projection of the Schwinger boson mean-field ground state. It is well known that such an RVB wavefunction can describe both the magnetic ordered and the quantum disordered state. Thus, it has the potential to provide an unbiased description of the quantum phase transition in BHM. The same type of variational wavefunction has been successfully applied to the study of the single-layer two-dimensional Heisenberg model [11, 13]. However, for the BHM, the variational calculation in [14] using such a wavefunction predicts a critical coupling \( \alpha_c \approx 3.51 \), which is a very bad estimate compared to the result of numerical simulation. A central issue to be addressed in this paper is to understand why the bosonic RVB state, which works so well on square lattices, fails for the BHM and how to improve it.

In this paper, we propose an RVB-type variational wavefunction with two variational parameters for the BHM. Similar to [14], our wavefunction is derived from the Gutzwiller projected Schwinger boson mean-field state. However, in our theory the intralayer RVB pairing and interlayer RVB pairing are treated as two independent variational parameters, rather than been determined by mean-field self-consistent equations. We find our variational wavefunction provides an accurate description of the quantum phase transition of the BHM. We find the transition is continuous. By analyzing the spin structure factor, ground state fidelity susceptibility and Binder moment ratio \( Q_4 \), the critical coupling strength is estimated to be \( \alpha_c \approx 2.62 \), in good agreement with those determined from the numerical simulation. The critical exponent estimated from the scaling analysis of the \( Q_4 \) data is also consistent with that of the classical 3D Heisenberg universality class.

Our result indicates that the bosonic RVB wavefunction derived from the Gutzwiller projection of the Schwinger boson mean-field state provides an accurate description of the quantum phase transition in quantum antiferromagnets. We also find that the failure of the Schwinger boson mean-field theory originates from the overestimation of the tendency to form interlayer dimers, which is again caused by the relaxation of the no-double-occupancy constraint. We have also calculated the fidelity susceptibility of the bosonic RVB wavefunction for the first time and find it a good indicator for the critical point of a quantum phase transition.

This paper is organized as follows. In section 2, we introduce the BHM and the bosonic RVB wavefunction. In section 3, we present the numerical method to perform calculations on such wavefunctions. In section 4, we present the numerical results and determine the critical point of the phase transition by analyzing the results of fidelity susceptibility and Binder moment ratio. In section 5, we present a discussion on related issues and conclude this paper.

2. The bilayer Heisenberg model and the RVB-type variational wavefunction

The model (BHM) we study in this paper is given by

\[
H = J_\parallel \sum_{\langle i,j \rangle, \mu} \hat{S}^\dagger_i \mu \cdot \hat{S}^\mu_j + J_\perp \sum_i \hat{S}^{\uparrow}_i \cdot \hat{S}^{\downarrow}_i,
\]

where \( \hat{S}_i^{\uparrow}, \hat{S}_i^{\downarrow} \) denote the spin operator at site \( i \) of layer \( \mu \) (\( \mu = 1, 2 \)), \( \sum_{\langle i,j \rangle} \) means the summation over nearest-neighboring sites on the square lattice of each layer. \( \alpha = J_\perp / J_\parallel \) is the only dimensionless parameter of the model. When \( \alpha = 0 \), the model describes two decoupled two-dimensional Heisenberg models, each of which are antiferromagnetic ordered at zero temperature. When \( \alpha \to \infty \), the system reduces to \( N \) decoupled interlayer dimers and the system is in a trivial quantum disordered state. A continuous quantum phase transition connects these two limits. Earlier numerical simulation shows that the phase transition occurs around \( \alpha_c = 2.52 \) [7, 8].

The bosonic RVB wavefunction we will adopt in this study is made of the coherent superposition of spin singlet configurations on the lattice and can be written as

\[
|\text{RVB}\rangle = \sum_{\{i_k, j_k\}} A(\{i_k, j_k\}) \prod_{k=1}^{N/2} S(i_k, j_k),
\]

in which \( S(i_k, j_k) = \frac{1}{\sqrt{2}} (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j) \) denotes the spin singlet pair between site \( i_k \) and \( j_k \). \( A(\{i_k, j_k\}) \) are the coefficients of the coherent superposition. In our case, \( A(\{i_k, j_k\}) \) can be written in a factorizable form \( A(\{i_k, j_k\}) = \prod_{k=2}^{N/2} A_{i_k, j_k} \).

The wavefunction equation (2) can be used directly as a variational state for quantum antiferromagnets. A more efficient and intuitively more attractive way to generate the RVB wavefunction is by Gutzwiller projection of the Schwinger boson mean-field state. This approach is used to study the two-dimensional Heisenberg model and has proved to be very successful. However, direct application of the approach to the BHM leads to unsatisfactory results.

Here, we will adopt the form of the Gutzwiller projected Schwinger boson mean-field state, but regard the mean-field order parameters (intralayer and interlayer RVB pairing amplitudes) as free variational parameters, rather than being determined from the mean-field self-consistent equations. The reason for such a choice is as follows. In the mean-field treatment, the no-double-occupancy constraint is relaxed. As a result, the quantitative prediction of the mean-field theory is not reliable. For example, the mean-field equation predicts an unphysical dimerization transition for BHM at \( \alpha \approx 4.62 \), whose origin can be traced back to the overestimation of the tendency to form interlayer dimers, which is again related to the relaxation of the local constraint.
In the Schwinger boson representation [4], the spin operator is written as

\[ \tilde{S} = \frac{1}{2} \sum_{\alpha, \beta = 1, 2} b^\dagger_{\alpha} \tilde{\sigma}_{\alpha, \beta} b^{}_{\beta}, \]  

(3)

in which \( b_{\alpha} \) is a boson operator and \( \tilde{\sigma} \) is the Pauli matrix. Equation (3) is a faithful representation of the spin algebra provided that the bosonic particle satisfies the no-double-occupancy constraint

\[ \sum_{\alpha} b^\dagger_{\alpha} b^{}_{\alpha} = 1. \]  

(4)

The BHM written in terms of the Schwinger boson operators is

\[ H = -J_i \sum_{\langle i, j \rangle, \mu} \hat{\lambda}_{i, j}^\mu \hat{\lambda}_{i, j}^{\mu \dagger} - J_\perp \sum_i \hat{\lambda}_i^\dagger \hat{\lambda}_i - \sum_{i, \mu} \lambda_{i, \mu} (n_{i, \mu} - 1) \]  

(5)

in which

\[ \hat{\lambda}_{i, j}^\mu = \frac{1}{\sqrt{2}} (b_{i, \mu, \uparrow} b_{j, \mu, \downarrow} - b_{i, \mu, \downarrow} b_{j, \mu, \uparrow}) \]

\[ \hat{\lambda}_i = \frac{1}{\sqrt{2}} (b_{i, \uparrow} b_{i, \downarrow} - b_{i, \downarrow} b_{i, \uparrow}) \]  

(6)

denote the intralayer and interlayer RVB pairing operator, \( n_{i, \mu} = \sum_{\alpha=\uparrow, \downarrow} b^\dagger_{i, \mu, \alpha} b^{}_{i, \mu, \alpha} \). The Lagrange multiplier \( \lambda_{i, \mu} \) is introduced to keep track of the local constraint.

In the mean-field theory, we treat \( \lambda_{i, \mu} = \lambda \) as a constant and decouple the interaction term using the following mean-field order parameters \( \Delta_{\parallel} = \langle \hat{\lambda}_{i, j}^{\mu \dagger} \rangle = \langle \hat{\lambda}_{i, j}^{\perp} \rangle \) and \( \Delta_{\perp} = \langle \hat{\lambda}_i^{\dagger} \rangle \). The mean-field Hamiltonian is (up to a constant)

\[ H_{\text{MF}} = -J_i \sum_{\langle i, j \rangle, \mu} \langle \hat{\lambda}_{i, j}^{\mu \dagger} \rangle b^\dagger_{i, \mu, \uparrow} b_{j, \mu, \downarrow} + \Delta_{\perp} \sum_i \hat{\lambda}_i^{\dagger} \hat{\lambda}_i - \lambda \sum_{i, \mu} n_{i, \mu}. \]  

(7)

The mean-field ground state of equation (7) is

\[ |G\rangle = \exp \left[ \sum_{\langle i, j \rangle, \mu, \nu} a_{i, \mu, j, \nu} (b^\dagger_{i, \mu, \uparrow} b_{j, \mu, \downarrow} - b^\dagger_{i, \mu, \downarrow} b_{j, \mu, \uparrow}) \right] |0\rangle, \]  

(8)

in which \(|0\rangle\) denotes the vacuum of the Schwinger boson. \( a_{i, \mu, j, \nu} \) represents the RVB amplitude between site \( i \) in the \( \mu \) layer and site \( j \) in the \( \nu \) layer. As a result of the bipartite nature of the system, the RVB amplitude is nonzero only for sites belonging to different sublattices. Thus for \( \mu = \nu \), \( a_{i, \mu, j, \nu} \) is nonzero only when \( i, j \) have different parities, while for \( \mu \neq \nu \) the reverse is true. The intralayer and interlayer RVB amplitudes are given by \( a_{i,1, j,1} = a_{i,2, j,2} = a_{i,2, j,1} \) by symmetry

\[ a_{i,1, j,1} = \frac{1}{N} \sum_k [\xi(k) + \eta(k)] \exp(ik \cdot r_{i,j}) \]

\[ a_{i,1, j,2} = \frac{1}{N} \sum_k [\xi(k) - \eta(k)] \exp(ik \cdot r_{i,j}), \]  

in which

\[ \xi(k) = \frac{c_1 \gamma(k) + c_2}{1 + \sqrt{1 - (c_1 \gamma(k) + c_2)^2}} \]

\[ \eta(k) = \frac{c_1 \gamma(k) + c_2}{1 + \sqrt{1 - (c_1 \gamma(k) - c_2)^2}}, \]  

here \( c_1 = 4J_1/\sqrt{2}c_2 = J_\perp \Delta_{\perp}/\sqrt{2}c_2, \gamma(k) = (\cos(k_x) + \cos(k_y))/2 \).

The bosonic RVB wavefunction adopted in this study is given by the Gutzwiller projection of the mean-field ground state into the physical subspace satisfying the local constraint

\[ |G\rangle = P_G \left[ \sum_{\langle i, j \rangle, \mu, \nu} a_{i, \mu, j, \nu} (b^\dagger_{i, \mu, \uparrow} b_{j, \mu, \downarrow} - b^\dagger_{i, \mu, \downarrow} b_{j, \mu, \uparrow}) \right] |0\rangle. \]  

(10)

Here \( P_G \) denotes the Gutzwiller projection and \( N \) is the number of lattice sites. The mean-field ground state contains two dimensionless parameters, namely \( c_1 \) and \( c_2 \). In the mean-field theory, both of them are determined by the mean-field self-consistent equations. Here we regard them as two independent variational parameters. This is the key difference between our theory and that of [14].

The proposed wavefunction equation (10) can describe both the magnetic ordered and the quantum disordered state. In equation (9), as \( c_1 + c_2 \to 1 \), both \( a_{i,1, j,1} \) and \( a_{i,1, j,2} \) become long-ranged and the wavefunction describes a state with antiferromagnetic long range order. On the other hand, when \( c_1 + c_2 \) deviates from 1, the RVB amplitudes \( a_{i,1, j,1} \) and \( a_{i,1, j,2} \) become short-ranged and the corresponding wavefunction describes a quantum disordered state. In fact, \( c_1 + c_2 = 1 \) is nothing but the Bose condensation condition in the mean-field theory. More specifically, when \( c_1 + c_2 = 1 \), both \( a_{i,1, j,1} \) and \( a_{i,1, j,2} \) decay with a power law of the form \( r_{ij}^{-3} \) at large distance, while when \( c_1 + c_2 < 1 \) both of them decay exponentially. As an illustration, we plot in figure 1 the RVB amplitudes as functions of distance for several values of \( c_1 + c_2 \) (the value of \( c_1 - c_2 \) is fixed at 0.2, which is close to its value at the transition point). The \( r_{ij}^{-3} \) decay of \( a_{i,1, j,1} \) and \( a_{i,1, j,2} \) at \( c_1 + c_2 = 1 \) is illustrated in figure 2.

On general grounds, we expect the interlayer pairing \( c_2 \) to decrease with \( \alpha \) and the intralayer pairing \( c_1 \) to decrease with \( \alpha \). The transition between the antiferromagnetic ordered state and the quantum disordered state is signaled by the deviation of \( c_1 + c_2 \) from 1. These expectations are confirmed in the numerical calculation.

### 3. The numerical techniques

The bosonic RVB wavefunction equation (10) can be studied by the standard loop gas Monte Carlo algorithm [12]. In this algorithm, the calculation of the expectation value of
a physical quantity $\hat{A}$ (for example, the energy) is done as follows:

$$
\frac{G(\hat{A})}{G(G)} = \frac{\sum_{\gamma,\gamma'} \psi_{\gamma}^* \psi_{\gamma'} \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle}{\sum_{\gamma,\gamma'} \psi_{\gamma}^* \psi_{\gamma'} \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle}.
$$

(11)

Here $|\gamma\rangle$ denotes the valence bond basis vector and is given by $|\gamma\rangle = \prod_{(i,j)\in V} S(i,j)$. $\psi_{\gamma}$ is the corresponding amplitude and is given by $\psi_{\gamma} = \prod_{(i,j)\in V} a_{i,j}$. The overlap between two valence bond basis vectors $|\gamma\rangle$ and $|\gamma'\rangle$ can be graphically interpreted as a loop gas on the lattice by fusing the valence bonds in the two basis vectors. It is easy to show that $\langle \gamma | \gamma' \rangle = 2^{N_L}$, where $N_L$ is the number of loops in the transition graph between $|\gamma\rangle$ and $|\gamma'\rangle$.

As the system is bipartite, the RVB amplitude $a_{i,j}$ and $a_{i,j}$ are, in fact, positive definite and the wavefunction equation (10) satisfy the Marshall sign rule [12]. For this reason, we can interpret $W(\gamma, \gamma') = \psi_{\gamma}^* \psi_{\gamma'} \langle \gamma | \gamma' \rangle$ as a normalized probability in the space of loop gas and can draw samples on it with the standard Monte Carlo method. The calculation of $\langle \gamma | \gamma' \rangle$ is easy for $\hat{A} = \vec{S}_i \cdot \vec{S}_j$ and the result is

$$
\langle \hat{A} \rangle = \sum_{\gamma,\gamma'} \psi_{\gamma}^* \psi_{\gamma'} \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle \langle \gamma | \gamma' \rangle.
$$

(12)

Thus both the energy and spin structure factor can be easily calculated with the standard Monte Carlo procedure in the loop gas space.

To determine the optimal value of the variational parameter $c_1$ and $c_2$, we calculate the expectation value of the energy and of its gradients in the parameter space $(c_1, c_2)$ on a finite lattice. It is useful to note that the gradients of energy can also be directly simulated by the loop gas Monte Carlo method. Its expression is given by

$$
\frac{\partial E(c_1, c_2)}{\partial c_{1,2}} = \left( \sum_{(i,j)\in V} \frac{\partial \ln a_{i,j}}{\partial c_{1,2}} \right) \langle \gamma | \hat{H} | \gamma' \rangle \rangle_L - E(c_1, c_2) \sum_{(i,j)\in V} \frac{\partial \ln a_{i,j}}{\partial c_{1,2}} \langle \gamma | \gamma' \rangle \rangle_L,
$$

(13)

where $\langle \cdot \rangle_L$ denotes the average over the loop gas configurations with the weight $W(\gamma, \gamma')$. We have used $10^8$ samples to calculate the energy and its gradients to determine the optimized values for $c_1$ and $c_2$. The boundary condition of the finite lattice is set to be periodic in both directions. The calculation is done on a lattice with sizes up to $20 \times 20 \times 2$, at which we find the critical coupling converges to $\alpha_c \approx 2.62$.

4. The numerical results

The optimized value for the parameter $c_1$ and $c_2$ as functions of the coupling constant $\alpha$ are shown in figure 3. As $\alpha$ increases, the interlayer RVB pairing strength $c_2$ increases at the expense of the intralayer RVB pairing strength $c_1$. The
Figure 3. The optimized value for the intralayer and interlayer RVB pairing strength $c_1$ and $c_2$ as functions of the coupling constant $\alpha$.

Figure 4. The optimized value for the variational parameter $a = c_1 + c_2$, which controls the order–disorder transition of BHM.

result is obtained on a $20 \times 20 \times 2$ lattice. It is found that the optimized values deviate significantly from the mean-field predictions, especially for large values of $\alpha$. For example, the mean-field theory predicts that $1/\perp$ would reach twice the value of $1/\parallel$ around $\alpha = 4$. However, the variational theory predicts that $1/\perp$ is slightly smaller than $1/\parallel$ around $\alpha = 4$. Thus, the mean-field theory overestimates greatly the tendency to form an interlayer dimer at large $\alpha$.

To better understand the evolution of the variational parameters as functions of $\alpha$, we plot the value of $a = c_1 + c_2$ as a function of $\alpha$ in figure 4. As we have shown above, the quantum phase transition between the magnetic ordered state and the quantum disordered state in our variational theory is solely controlled by the value of $\alpha$. The value of $a$ is seen to deviate from unity around 2.6, at which the Bose condensate of the spinon is gone.

To further characterize the quantum phase transition and determine the value of the critical coupling $\alpha_c$, we study the following three kinds of quantities: the spin structure factor at the ordering wavevector, the fidelity susceptibility of the ground state and the Binder moment ratio $Q_2$.

4.1. Spin structure factor

For a finite system, the spontaneous magnetization can be defined in a spin-rotational-invariant way as the square root of the spin structure factor at the magnetic Bragg vector. For BHM, the Bragg vector is $\vec{Q} = (\pi, \pi, \pi)$. The spin structure factor is defined as

$$S(\vec{q}) = \frac{1}{N} \sum_{i,j} \langle \vec{S}_i \cdot \vec{S}_j \rangle \exp(i\vec{q} \cdot \vec{r}_{ij}).$$

For $q = Q$, we have

$$M^2 = NS(\vec{Q}) = \sum_{i,j} (-1)^{i-j} \langle \vec{S}_i \cdot \vec{S}_j \rangle.$$ (15)

In the quantum disordered state, as the spin correlation length is finite, $S(\vec{Q})$ is of order one. However, in the magnetic ordered state, $S(\vec{Q})$ should scale like $N$ and thus $M$ is an extensive quantity.

The result of the spin structure factor for a $20 \times 20 \times 2$ system is shown in figure 5. An order–disorder transition can be seen around 2.5. However, the signature of a phase transition in the spin structure factor is not sharp enough for an accurate determination of the critical coupling strength. The transition is rounded into a crossover as a result of the finite size effect. For this reason, we need some other quantities that are more sensitive to the transition to determine the critical coupling.

4.2. Fidelity susceptibility

The concept of fidelity susceptibility is introduced to describe the sensitivity of the ground state to the variation of the parameters in Hamiltonian $[9]$ and is expected to reach its maximum at the critical coupling of a quantum phase transition, where the ground state is the most susceptible to the variation of the controlling parameters of the phase transition. The fidelity susceptibility is defined in the following manner for a system with only one parameter $\alpha$:

$$\chi_f = -2 \lim_{\delta \alpha \to 0} \ln |\langle O(\alpha, \delta \alpha) | (\delta \alpha)^2 |,$$ (16)
in which $O(\alpha, \delta \alpha) = \langle \Psi_0 | \Psi_{\alpha + \delta \alpha} \rangle$ denotes the overlap between the normalized ground state vector for parameter values $\alpha$ and $\alpha + \delta \alpha$.

In our variational theory, the fidelity susceptibility can be calculated directly. We first fit the optimized variational parameters as functions of $\alpha$ and then calculate the overlap between variational ground states for nearby values of $\alpha$. The overlap between the bosonic RVB states is calculated in the following way:

$$\frac{\langle \Psi | \Psi' \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_{y, y'} \psi_y^* \psi_{y'} \langle \gamma | y' \rangle \langle y' | \gamma' \rangle}{\sum_{y, y'} \sum_{y'} \psi_y^2 \psi_{y'}^2 \langle \gamma | y' \rangle \langle y' | \gamma' \rangle}. \quad (17)$$

In our calculation, we have set $\delta \alpha = 0.01$. The result for the fidelity susceptibility for systems of several sizes is shown in figure 6. A pronounced peak appears around $\alpha = 2.6$. Figure 7 shows the peak position extracted from figure 6 as a function of the system size $L$. It is found that the peak position converges rapidly to its thermodynamic limit value $\alpha_c \approx 2.62$ when $L > 10$.

### 4.3. Binder moment ratio $Q_2$

To confirm the result derived from the fidelity susceptibility, we calculate the Binder moment ratio $Q_2$ [8, 10]. The Binder moment ratio $Q_2$ is a dimensionless quantity defined in the following manner:

$$Q_2 = \frac{\langle \hat{S}_Q^2 \rangle}{\langle \hat{S}_Q \rangle^2}, \quad (18)$$

in which $\hat{S}_Q = \sum_{i,j} (-1)^{i+j} \hat{S}_i \cdot \hat{S}_j$. Note our definition of $Q_2$ is slightly different from the standard one in that it is defined in a spin-rotational-invariant way, while in the standard definition only the $z$ component of the moment is used. The Binder moment ratio is very useful in the analysis of the critical properties as it is universal near the critical point. More specifically, it can be expressed as a universal scaling function of $tL^{1/v}$, where $t = (\alpha - \alpha_c)$ and $v$ is the critical exponent for correlation length.

The results of $Q_2$ for system with $L = 14, 16, 18$ and 20 are shown in figure 8. It is found that all curves cross with each other at approximately the same value of $\alpha$, in accordance with the scaling hypothesis. The estimated value of the critical coupling strength is $2.62$, in good agreement with that estimated from the fidelity susceptibility data. The $Q_2$ value at the crossing point is found to be approximately 1.23, close to but smaller than the value (1.29) estimated from the quantum Monte Carlo simulation with the standard definition of $Q_2$. Such a difference may be caused by the difference in the definitions of $Q_2$.

Figure 9 shows the scaling of the $Q_2$ data with the scaling form $Q_2 = M(tL^{1/v})$, where $t = (\alpha - \alpha_c)$ and $v$ is the exponent for the correlation length. The best fit is reached by $\alpha_c \approx 2.62$ and $1/v \approx 1.4$. The critical exponent so obtained $v \approx 0.714$ is thus quite close to the result of the quantum Monte Carlo simulation.
5. Conclusion

In this work, we proposed a bosonic resonating valence bond (RVB) wavefunction with the form of the Gutzwiller projected Schwinger boson mean-field ground state for the BHM. We find the proposed wavefunction predicts a continuous phase transition between the antiferromagnetic ordered state and the quantum disordered state. To determine the critical coupling strength, we have calculated the spin structure factor, the fidelity susceptibility and the Binder moment ratio \( Q_2 \). Through finite size scaling analysis of the latter two quantities, we find the critical coupling to be given by \( \alpha_c \approx 2.62 \), in good agreement with the quantum Monte Carlo simulation results. The scaling analysis of \( Q_2 \) also provides an estimate of the correlation length critical exponent \( (1/\nu \approx 1.4) \), which is also in good agreement with the results of quantum Monte Carlo simulation. We find the intralayer correlation is quite large at the phase transition point and it dominates over the interlayer correlation for \( \alpha \) twice as large as the critical coupling strength. Thus, the ground state of the system at \( \alpha = \alpha_c \) is far away from the limit of independent dimer states. The discontinuous transition to such a dimerized state in the mean-field theory should thus be an artifact.

Our work indicates that the bosonic RVB wavefunction derived from the Gutzwiller projection of the Schwinger boson mean-field ground state has the potential to capture the physics of quantum phase transitions with high accuracy. The failure of it in a previous variational study [14] can be attributed to the weakness of the mean-field theory, which overestimate the tendency of the system to form interlayer dimers. Such an overestimation is closely related to the relaxation of the local constraint in the mean-field treatment, which prohibit multiple occupation of a dimer on a given bond, even if the mean-field theory points to the tendency of Bose condensation of such interlayer dimers. The same instability also causes the failure of the mean-field theory itself for large \( \alpha \). Hence, the form of the ground state predicted by the mean-field theory is correct: however, the quantitative relation between mean-field order parameters is less meaningful. The local constraint is thus indispensable for a correct description of the quantum antiferromagnet with the bosonic RVB state.

In this work, we have proved the usefulness of the variational approach to the quantum phase transition in BHM. However, a more detailed study of the critical behavior and the excitation spectrum around the critical point is obviously needed to further characterize the quantum critical point in this system. We will leave this task to future investigations.

Acknowledgments

This work is supported by the NSFC grant no. 10774187 and the National Basic Research Program of China nos 2007CB925001 and 2010CB923004. The authors acknowledge the discussion with Yizhuang You on fidelity susceptibility.

References

[1] Sachdev S 1999 Quantum Phase Transitions (Cambridge: Cambridge University Press)
[2] Matsuda T and Hida K 1990 J. Phys. Soc. Japan 59 2223
[3] Shevechenko P V and Sushkov O P 1999 Phys. Rev. B 59 8383
[4] Kotov V N, Sushkov O, Weihoang Z and Oitmaa J 1998 Phys. Rev. Lett. 80 5790
[5] Arovas D P and Auerbach A 1988 Phys. Rev. Lett. 61 316
[6] Millis A J and Monien H 1993 Phys. Rev. Lett. 70 2810
[7] Wang L, Beach K S D and Sandvik A W 2006 Phys. Rev. B 51 16606
[8] Collins A and Hamer C J 2008 Phys. Rev. B 78 054419
[9] Sachdev S and Bhatt R N 1990 Phys. Rev. B 41 9323
[10] Chubukov A V and Morr D K 1995 Phys. Rev. B 52 3521
[11] Millis A J and Monien H 1994 Phys. Rev. B 50 16606
[12] Weihong Z 1997 Phys. Rev. B 55 12267
[13] Hida K 1990 J. Phys. Soc. Japan 59 2230
[14] Gelfand M P 1996 Phys. Rev. B 53 1130
[15] Sandvik A W and Scalapino D J 1994 Phys. Rev. Lett. 72 2777
[16] Sandvik A W and Scalapino D J 1996 Phys. Rev. B 53 R526
[17] Sandvik A W, Chubukov A V and Sachdev S 1995 Phys. Rev. B 51 16483
[18] Wang L, Beach K S D and Sandvik A W 2006 Phys. Rev. B 73 014431
[19] Zanardi P and Paunkovic N 2006 Phys. Rev. E 74 031123
[20] Gellert K 1981 Phys. Rev. Lett. 47 693
[21] Liang S, Doucot B and Anderson P W 1988 Phys. Rev. Lett. 61 153
[22] Anderson P W 1973 Mater. Res. Bull. 8 153
[23] Chen Y and Xiu K 1993 Phys. Rev. B 35 1373
[24] Miyazaki T, Nakamura I and Yoshioka D 1996 Phys. Rev. B 53 12206