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Ground-State Behavior of the Quantum Compass Model in an External Field *

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Ground-state (GS) properties of the two-dimensional (2D) quantum compass model in an external field on a square 5×5 lattice are investigated by using the exact diagonalization (ED) method. We obtain the GS energy and evaluate quantities such as its correlation functions, nearest-neighbor entanglement and local order parameter. As the external field is presented, the first-order quantum phase point is absent and the system exhibits the behaviors of the second-order phase transition.

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Recently, properties of the orbital compass models have attracted considerable attention for so-called dimensional reduction.[1,2] As a simple model of orbital order in the transition-metal oxide compounds, the quantum compass model has been studied extensively.[3–9] It was first introduced for determining the physics of Mott insulators with orbital degrees of freedom and the implementation of protected qubits for quantum computation in Josephson junction arrays.[5] Furthermore, it can also describe polar molecules in optical lattices and systems of trapped ions.[10,11] The one-dimensional (1D) compass model is exactly solvable and shows the same universality class as the 1D transverse-field Ising.[12–15] The compass model on a 2D square lattice is described as the coupling between spin components on neighboring lattice sites, which is tied to the direction of the corresponding bonds, with Ising-like interactions $J_x\sigma_i^x\sigma_{i+e_{\hat{x}}}^x$ and $J_z\sigma_i^z\sigma_{i+e_{\hat{z}}}^z$ along the $\hat{x}$ and $\hat{z}$ axes of the lattice.[9,16] It describes all non-local compass excitations over the GS while the local ones manifest themselves by directions of symmetry-breaking fields.[9] However, the exact solution of the 2D compass model has not been obtained yet. Some recent numerical calculation results show that the phase transition in the anisotropic quantum orbital compass model on a square lattice is of the first order.[8,16–18] In addition, the thermal canting effect in the x–z plane of the 2D quantum compass model in a magnetic field was reported in Ref. [19] by using the Monte Carlo method.

The extension to finite field is a crucial step in the search for systems supporting naturally robust quantum information. Generally speaking, the symmetry of the system is further broken when a magnetic field is applied. The behavior of the energy gap may be changed around a critical point in the thermodynamical limit.[15] Accordingly, the nature of the quantum phase transition (QPT) may also be altered. In this Letter, we employ the ED method to calculate the GS properties of the transverse field compass model on a square 5×5 lattice with the periodic boundary condition (PBC). The numerical results show that the 2D quantum compass model in an external magnetic field will exhibit behaviors of a second-order phase transition and the phase transition point is decided by the external field.

When considering an external magnetic field, the Hamiltonian of the 2D compass model on a square $L \times L$ lattice with the PBC is given by

$$H = -J_x \sum_{i,j=1}^{L} \sigma_{i,j}^x \sigma_{i+1,j}^x - J_z \sum_{i,j=1}^{L} \sigma_{i,j}^z \sigma_{i,j+1}^z - \frac{h}{2} \sum_{i,j=1}^{L} \sigma_{i,j}^z, \tag{1}$$

where $\{\sigma_{i,j}^x, \sigma_{i,j}^z\}$ are the Pauli matrices at site (i,j), the coupling strengths J_x, J_z in Eq. (1) are restricted to the range $[0,1]$ and written in terms of a variable $s \in [0,1]$ as $J_x = \cos(s\pi/2)$, $J_z = \sin(s\pi/2)$ for convenience, i (j) is a vertical (horizontal) index, h is the transverse magnetic field. For $s = 0$, the Hamiltonian (1) is decoupled as the 1D transverse field Ising model which is a quantum model. For $s = 1$, the compass model is decoupled as a 1D classical model. In the case of L being even, the model is equivalent to the antiferromagnetic quantum compass model. The exact solution of the 2D compass model has not been found at present. To obtain some meaningful results, we employ the ED method to explore the GS properties of the system. It is possible to perform ED (Lanczos) of 2D $L \times L$ clusters up to $L = 5(L = 6)$ by using the symmetry operators of the Hamiltonian. Firstly, we focus on the case of $h = 0$. Thus the Hamiltonian H in Eq. (1) has a set of $2L$ operators $\{P_i, Q_j\}$ which are defined for $i, j = 1, 2, \cdots, L$ as

$$P_i = \prod_{j=1}^{L} \sigma_{i,j}^x, \quad Q_j = \prod_{i=1}^{L} \sigma_{i,j}^z. \tag{2}$$

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One can identify that both operators commute with the Hamiltonian ($h = 0$) and anticommute with one another. Moreover, the commute relation $[P_i P'_i, Q_j] = [P_i, Q_j Q'_j] = 0$ is also satisfied.[5,8] The symmetry operators $Q(P)$ result in a two-fold degeneracy of each chain, so a massive GS degeneracy of the 2D system achieves at least 2^L. The Hamiltonian can be diagonalized in the subspace which is constructed with $\{p_i\}$ and $\{r_j\}$, where $p_i = \pm 1$ and $r_j = \pm 1$ are the eigenvalues of the operators P_i with $i = 1, 2, \ldots, L$ and $R_j = Q_j Q_{j+1}$ with $j = 1, 2, \ldots, L-1$, respectively. Thus the Hamiltonian can be written in terms of $(L-1) \times (L-1)$ new spin operators and $L \times (L-1)$ parameters $\{p_i\}$ and $\{r_j\}$ can construct $2^{2\,L-1}$ subspaces.[17] When the external magnetic field is considered, the symmetry of system is broken. The symmetry operators Q_j are still available, which commute with the Hamiltonian (1), i.e. Q_j's eigenvalues are the good quantum numbers. Then the Hilbert space of the Hamiltonian can only be decreased as 2^{L^2-L}. For the ED method, the maximum cluster size is possibly up to $L = 5$ in this case.

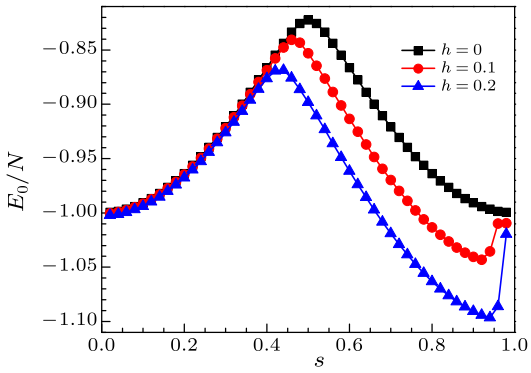

Fig. 1. (Color online) The average GS energies for $h = 0, 0.1, 0.2$ as a function of parameter s on a square 5×5 lattice.

To study the properties of QPT, the GS needs to be obtained. Both the GSs of Hamiltonian (1) with no external field in subspace $\mathcal{H}_1 \equiv \mathcal{H}(I_1 = -1, I_2 = -1, \ldots, I_L = -1)$ and $\mathcal{H}_2 \equiv \mathcal{H}(I_1 = 1, I_2 = 1, \ldots, I_L = 1)$ have the lowest energy E_0, where $\mathcal{H}(I_1, I_2, \ldots, I_L) = \mathcal{H}_1^{I_1} \otimes \mathcal{H}_2^{I_2} \otimes \cdots \otimes \mathcal{H}_L^{I_L}$, and $\mathcal{H}_l^{-1}$ ($\mathcal{H}_l^1$) denotes the subspace $\mathcal{H}_l^{\rm odd}$ ($\mathcal{H}_l^{\rm even}$). The two subspaces $\mathcal{H}_l^{\rm odd}$ and ($\mathcal{H}_l^{\rm even}$) are decided by the parity of pseudospin number M_l, where $M_l \equiv m_{l,1} + m_{l,2} + \cdots + m_{l,L}$ and $m_{l,k}$ represent the eigenvalue of the pseudospin z-component operator.[20] For $h \neq 0$, Hamiltonian (1) can still be divided into the two subspaces $\mathcal{H}_l^{\rm odd,even}$ because the operators $\sigma_{i,j}^z$ commute with Q_j. However, the degeneracy of the subspaces $\mathcal{H}^{\rm odd,even}$ is eliminated. The global GSs of the 2D compass model are destroyed in the presence of the external magnetic field.

The numerical results of the GS behaviors on a square 5×5 lattice are obtained and analyzed by using the ED method. The PBC is assumed. Firstly, the average GS energies for different external fields are obtained in Fig. 1. For $h = 0$, the result is very similar to Ref. [16], but the sharp peak with a discontinuous derivative is not obvious due to the limits of system size. The average GS energy (i.e., E_0/N, where N is the lattice number of the system) decreases with the increase of the magnetic field. It is obvious that the z direction field breaks the symmetry of energy versus parameter s. In addition, under the influence of the external field, the GS energy E_0 incurs an abrupt jump near $s = 1$ since the Hamiltonian (1) has transformed from a quantum one to a classical one at that point. It is found that the external field mainly affects the GS energy in the regime of $s > s_{\max}$ ($s_{\max}(h = 0.1) \simeq 0.46$ and $s_{\max}(h = 0.2) \simeq 0.43$), where one has $E_0(s_{\max}) = E_0^{\max}$.

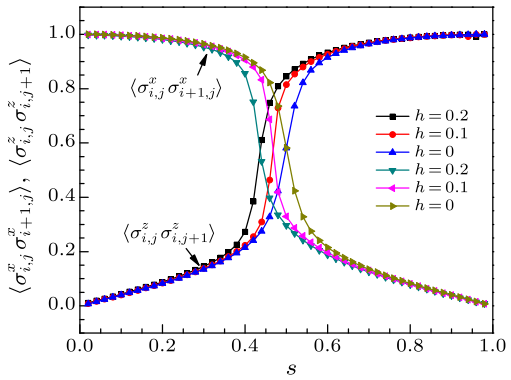

Fig. 2. (Color online) The nearest-neighbor GS correlation functions for $h = 0, 0.1, 0.2$ as a function of parameter s on a square 5×5 lattice.

The nearest-neighbor GS correlation functions $\langle\sigma_{i,j}^x \sigma_{i+1,j}^x\rangle$ and $\langle\sigma_{i,j}^z \sigma_{i,j+1}^z\rangle$ are also interesting physical quantities, as shown in Fig. 2. The effect of the external field on the correlation functions is concentrated in the middle regime of parameter s. The correlation functions for a different external field have cross points at $s_{\max}$. The QPT points usually correspond to the position of these cross points. However, the existence of the QPT may not be identified from this starting point.

For a better grasp of the nature of the QPT, we evaluate the order parameter $\langle\sigma^z\rangle \equiv \frac{1}{N}\sum_{i,j=1}^{L}\langle\sigma_{i,j}^z\rangle$, as shown in Fig. 3. The result for $h = 0$ is similar to Refs. [8,16] and an abrupt jump of the order parameter can be identified at $s = 0.5$. In the thermodynamic limit, the first-order QPT indeed occurs in the $h = 0$ case. However, whether the QPT exists in the presence of the external field is not readily decided by Fig. 3. For the sake of confirming the QPT point, we calculate the GS fidelity, which is defined as[21–26]

$$F(\alpha, \delta\alpha) = |\langle\psi_0(\alpha)|\psi_0(\alpha + \delta\alpha)\rangle|, \qquad (3)$$

where ψ_0 is the GS wave function obtained by using

the ED method, $\delta\alpha$ is a small quantity ($\delta\alpha = 10^{-4}$ is taken in the present calculation). One can identify the QPTs in various many-body systems from the GS fidelity. The GS fidelity decays to zero in the first-order QPT, while the scaling relation occurs in continuous phase transition systems. In the PBC, the abrupt jump point of the fidelity is basically invariable even though the size of system is altered.[15] The results for $h \neq 0$ are given in Fig. 4.

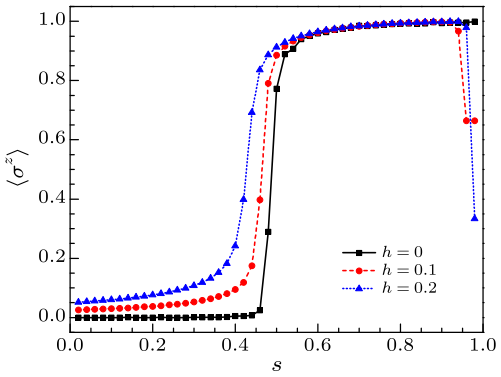

Fig. 3. (Color online) The order parameter for $h = 0, 0.1, 0.2$ as a function of parameter s on a square 5×5 lattice. The step function for $h = 0$ shows a discontinuous transition.

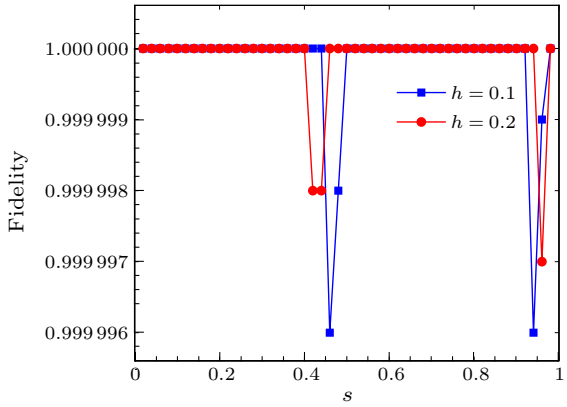

Fig. 4. (Color online) The GS fidelity for $h = 0.1, 0.2$ as a function of parameter s on a square 5×5 lattice.

It is found that the nontrivial QPT points become gradually further from $s = 0.5$ with the increase of the external field. The QPT point occurs exactly at $s_{\max}$. The other important problem is to find the relation of the QPT point $s_{\max}$ and the external field h. The linear relation is found, as shown in Fig. 5. The result is possibly established in the thermodynamic limit.

We then turn to the quantum entanglement of this system. The nearest-neighbor spin two-point correlation functions are used to calculate the nearest-neighbor concurrence (NNC) of the system. The concurrence is defined as $C(i,j) = \max[r_1(i,j) - r_2(i,j) - r_3(i,j) - r_4(i,j), 0]$, where $r_\alpha(i,j)$ are the square roots of the eigenvalues of the product matrix $R = \rho_{ij}\widetilde{\rho_{ij}}$ in descending order.[27–30] The spin flipped matrix $\widetilde{\rho_{ij}}$ is given by $\widetilde{\rho_{ij}} = (\sigma^y \otimes \sigma^y)\rho_{ij}^*(\sigma^y \otimes \sigma^y)$. The ρ_{ij}^* is the density matrix and has the form as follows:[28,29]

$$\rho_{ij} = \frac{1}{4}\sum_{\alpha,\beta=0}^{3} p_{\alpha\beta}\sigma_i^\alpha \otimes \sigma_j^\beta. \tag{4}$$

The coefficients are determined by the relations

$$p_{\alpha\beta} = tr(\sigma_i^\alpha \sigma_j^\beta \rho_{ij}) = \langle\sigma_i^\alpha \sigma_j^\beta\rangle. \tag{5}$$

The results are plotted in Fig. 6. The quantum entanglement appears in the range of $s > s_{\max}$. This behavior is also valid in the thermodynamic limit. It is worth noting that the NNC does not exhibit an obvious distinction for $h = 0$ and $h \neq 0$. The finite-size effect is more evident in the calculation of the NNC.

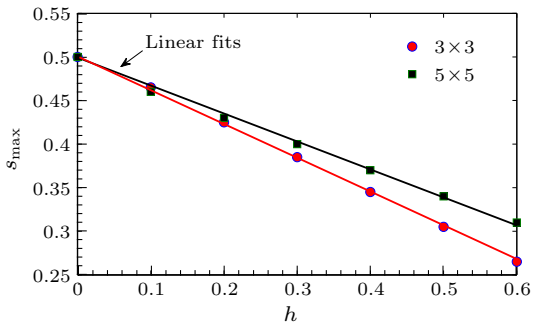

Fig. 5. (Color online) The QPT point $s_{\max}$ as a function of h on the square 3×3 and 5×5 lattices.

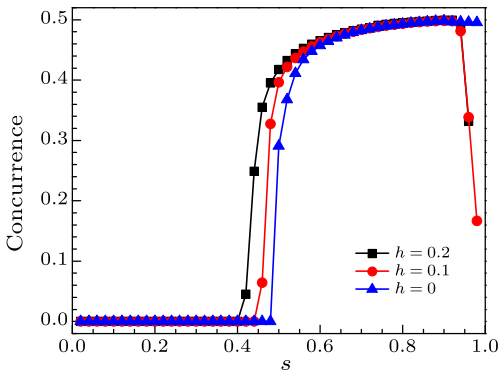

Fig. 6. (Color online) The NNC for $h = 0, 0.1, 0.2$ as a function of parameter s on a square 5×5 lattice.

The binder cumulant can usually be used to identify the phase transition temperature T_c. It is a standard tool in the study of second-order transitions.[31,32] Some authors have also advocated its use in the case of a KT-transition.[33,34] The prototype of such a quantity is the fourth-order cumulant of the magnetization and it is defined by

$$U(T,C) = 1 - \frac{M_C^{(4)}}{3(M_C^{(2)})^2}, \tag{6}$$

where C represents a spin cluster;[31,32] $\langle M^{(2)}\rangle_C$ and $\langle M^{(4)}\rangle_C$ denote the second and fourth moments of the magnetization in that cluster, which has the general

expression

$$M^{(k)} = \langle (\frac{1}{L^2} \sum_{i,j=1}^{L} \sigma_{i,j}^{z})^k \rangle, \quad (7)$$

taking thermal averages. Considering the zero temperature phase transition, the above thermal averages need be only amended as the GS averages. The GS binder cumulants are plotted in Fig. 7. The odd sizes are adopted for eliminating the difference of the GS properties of the system. It is found that the GS binder cumulants for different sizes ($L = 3, 5$) have a cross point which is just at the QPT point $s_{\max}$. Note that $s_{\max}$ does not change for different sizes in the PBC. Therefore we conclude that the binder cumulant for different lattice sizes should intersect at a point. However, the GS binder cumulant tends to the value 2/3 in the range of $s > s_{\max}$ and to zero in $s < s_{\max}$, as shown in Fig. 7. It is interesting that our results can be used to compare with the 2D square lattice Ising case. Specifically speaking, the cumulant for the Ising case approaches the thermodynamic limit value 2/3 at temperatures $T < T_c$, while it tends to zero, reflecting a Gaussian distribution of the magnetization histogram, at $T > T_c$.[31,32] Here we can infer that the parameter $s_{\max}$ in the QPT acts as the function of the transition temperature T_c. The similar results show that the 2D quantum compass model with a magnetic field is more likely to exhibit the properties of the second-order phase transition and the phase transition point is determined by the external field. However, at present, we cannot give the exact dependency relationship between the QPT and the external field since there is still no exact solution for the 2D quantum compass model.

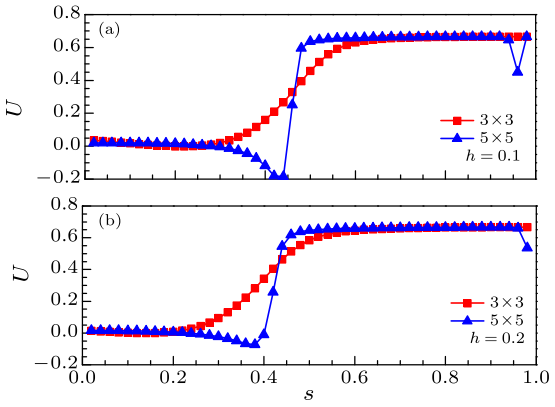

Fig. 7. (Color online) The GS binder cumulant as a function of parameter s for sizes $L = 3, 5$, (a) for $h = 0.1$ and (b) for $h = 0.2$.

In summary, we have used the ED method to study the GS behaviors of the 2D quantum compass model in a magnetic field on a square 5×5 lattice with the PBC. The global GSs of the 2D compass model are destroyed in the presence of the external magnetic field. The first-order QPT is observed for $h = 0$, while the second-order QPT is confirmed in the case of $h \neq 0$ by comparing the binder cumulant with the 2D square lattice Ising model. It is found that the linear relation is satisfied between the phase transition point and the external field. However, the exact dependency relationship between the QPT and the external field is difficult to obtain.

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