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Effects of Heisenberg perturbation on the ground-state properties of one-dimensional extended quantum compass model

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ABSTRACT

The ground-state properties and quantum phase transitions (QPTs) of the one-dimensional extended quantum compass model (EQCM) with Heisenberg perturbation are investigated by the infinite time-evolving block decimation (iTEBD) algorithm. The ground-state properties are found to be affected distinctively by the Heisenberg perturbation and rich phase diagrams are obtained. The first-order QPTs line at $J_1 = 0$ disappears even with an infinitesimal Heisenberg perturbation and two interesting intermediate phases, such as a disordered phase and a transverse Néel phase, are induced. Both bipartite entanglement and fidelity per site are capable of describing all the second-order QPTs.

1. Introduction

The role of the orbital degrees of freedom in determining the magnetic and transport properties of transition metal oxides (TMOs) has been widely recognized [1–6]. The complex intrinsic interplay in TMOs induces various fascinating physical phenomena and extremely rich phase diagrams [7]. In order to mimic the orbital states with a two-fold degeneracy, the quantum compass model (QCM) was firstly introduced [8]. It was argued that materials with large spin–orbit coupling may give rise to compass spin interaction [9], leading to either the compass or the Kitaev honeycomb model [10]. Besides the ability to describe t_{2g} systems, the compass model also shows some interdisciplinary characters. Recently, it was proposed that the compass model can be used to describe the physics of protected qubits [11,12], so it may have potential application in quantum information techniques. Due to the strong quantum frustration in compass spin interaction, it is difficult to solve analytically. Furthermore, such an interaction may lead to large degeneracy in the energy spectrum and thus set obstacles for numerical simulations [13]. It was suggested generally that there should exist a symmetry-broken ground state and a first-order quantum phase transition (QPT) at the self-dual point [14–18]. Recently, one-dimensional (1D) QCM has triggered extensive studies [19–28]. By mapping to the quantum Ising model, Brzezicki et al. solved the 1D extended QCM (EQCM) exactly and observed a first-order QPT between two disordered phases [19]. Then, Eriksson and Johannesson [25] investigated the same model with more tunable parameters and suggested that the first-order transition in fact occurs at a multicritical point where a first-order transition line meets with a second-order transition line.

On the other hand, general perturbations might cause fundamental effects on the nonlocal characteristic of the compass model [11,14,29]. Recently, Trousselet et al. studied the compass model on the square lattice under the influence of perturbing Heisenberg interactions [30], as suggested by possible solid state applications [9,31]. It was shown that the ground-state degeneracy of the compass model is lifted in the thermodynamic limit by infinitesimal Heisenberg coupling and a rich phase diagram was presented with various quantum phase transitions between various phases of Z_2 symmetry [32].

In this paper, we would like to discuss the effects of the Heisenberg perturbation on the ground-state phase diagram of the 1D EQCM. Hereafter, the EQCM with Heisenberg perturbation is called the extended quantum compass Heisenberg model (EQCHM). By the infinite time-evolving block decimation (iTEBD) algorithm [33], the matrix product state (MPS) ground state can be obtained and some interesting quantities can be calculated. We would like to study the QPTs in such a model and obtain the ground-state phase diagram. As will be shown, the ground-state properties are affected distinctively by the Heisenberg perturbation and novel phases will be induced.

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2. Hamiltonian and numerical method

The 1D EQCHM is defined by

$$\hat{H} = \sum_{i=1}^{N'} (J_1 S_{2i-1}^z S_{2i}^z + J_2 S_{2i-1}^x S_{2i}^x + L_1 S_{2i}^z S_{2i+1}^z) + \sum_{j=1}^{N} J_H \hat{\mathbf{S}}_j \cdot \hat{\mathbf{S}}_{j+1}, \quad (1)$$

where $N = 2N'$ is the total number of sites and $\hat{\mathbf{S}} = (S^x, S^y, S^z)$ denotes a spin-1/2 operator. J_1 and J_2 on odd bonds and L_1 on even bonds are spin exchange couplings. The J_H denotes the isotropic Heisenberg perturbation. $L_1 = 1$ is set as an energy scale in our calculations. The ground-state phase diagram of 1D EQCHM without considering the Heisenberg perturbation was provided previously [25]. A first-order QPT line $J_1 = 0$ and a second-order QPT line $J_2 = 1$ were determined. Four different phases including two disordered regions I ($J_1 > 0$, $J_2 > 1$) and II ($J_1 < 0$, $J_2 > 1$), a stripe phase (SP) III ($J_1 < 0, J_2 < 1$), and a Néel phase (NP) IV ($J_1 > 0$, $J_2 < 1$) are separated by $J_1 = 0$ and $J_2 = 1$. Subsequently, the first-order QPT between regions I and II without energy level crossing, which was suggested to be an "accidental" exception, was detected by the fidelity and string order parameters [28].

The iTEBD method [33] is applied to obtain the ground state $|\psi_g\rangle$ by acting an imaginary time evolution operator $\exp(-\tau\hat{H})$ on an arbitrary initial state $|\psi_0\rangle$. The operator $\exp(-\delta\tau\hat{H})$ with small enough $\delta\tau$ is expanded into a sequence of two-site gates $U^{[i,i+1]}$ by a Suzuki-Trotter decomposition. In the limit $\tau \to \infty$, the resulting wave function $\exp(-\tau\hat{H})\,|\psi_0\rangle$ converges to the ground state $|\psi_g\rangle$ of $\hat{H}$. A four-period MPS

$$|\psi\rangle = \mathrm{Tr}\left(\prod_i^{N/4} \Lambda^a \Gamma_{4i-3}^a \Lambda^b \Gamma_{4i-2}^b \Lambda^c \Gamma_{4i-1}^c \Lambda^d \Gamma_{4i}^d\right) |m_{4i-3}, m_{4i-2}, m_{4i-1}, m_{4i}, \ldots\rangle \quad (2)$$

is adopted to describe the ground state. The Γ^α and Λ^α ($\alpha = a, \ldots, d$) represent three-indexed tensors and $\chi \times \chi$ diagonal matrices, respectively. To reduce the cutoff error, the bond dimension χ is set up to 60. Based on the ground-state wavefunction obtained by iTEBD, we can calculate some expected values by $\overline{O} = \langle\psi_g|\hat{O}|\psi_g\rangle$.

In addition, it has been shown that the quantum entanglement has close relation to the QPTs in many-body systems [34]. The von Neumann entropy as a bipartite entanglement measure is usually adopted [35] to describe the QPTs. By cutting a bond randomly, a spin chain will be partitioned into two parts, i.e., the left semi-infinite chain and the right semi-infinite chain. Given the MPS in its canonical form, bipartite entanglement S_b is defined as

$$\mathcal{S}_b = -\sum_i \Lambda_i^2 \log_2 \Lambda_i^2. \quad (3)$$

Four bipartite entanglement measures ($S_{4i-3,4i-2}$, $S_{4i-2,4i-1}$, $S_{4i-1,4i}$, and $S_{4i,4i+1}$) can be calculated.

Besides bipartite entanglement, the fidelity per site (f) can be defined by

$$\ln f = \lim_{N\to\infty} \frac{\ln\langle\psi_{\mathrm{ref}}|\psi_g\rangle}{N}, \quad (4)$$

which can be used to detect the QPTs [36]. The $|\psi_{\mathrm{ref}}\rangle$ denotes a reference state and $|\psi_g\rangle$ is the ground state. The f quantifies the overlap between $|\psi_g\rangle$ and $|\psi_{\mathrm{ref}}\rangle$.

3. Ground-state phase diagram and QPTs

In this section, four typical paths ($J_2 = 0.5$, $J_2 = 2$, and $J_1 = \pm 1$) will be chosen to discuss the effects of the Heisenberg perturbation.

First, we consider the QPTs along the line $J_2 = 0.5$. Without considering the Heisenberg perturbation ($J_H = 0$), a first-order QPT from SP (III) to the NP (IV) occurs at $J_1 = 0$. Once the Heisenberg perturbation is taken into account, we find that the first-order QPT

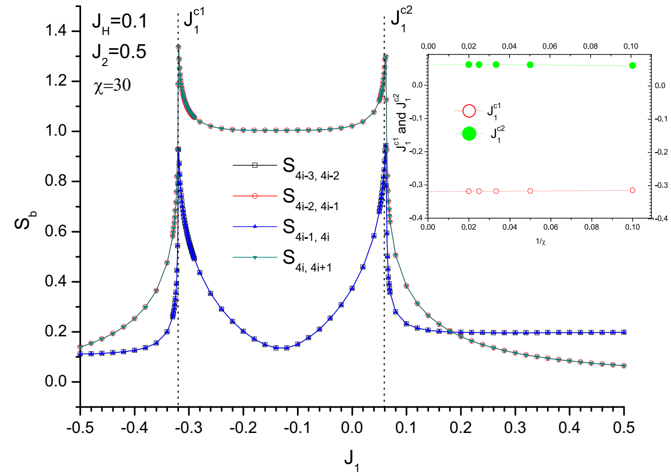

Fig. 1. (Color online) (a) Bipartite entanglement on different bonds exhibit two singularities at J_1^{c1} and J_1^{c2}. The inset shows the scaling of the two critical points versus the $1/\chi$.

point disappears and an intermediate phase is induced. To present our main results clearly, we just select $J_H = 0.1$ as an example. The bipartite entanglement versus varying J_1 is plotted in Fig. 1. Two distinct maxima at J_1^{c1} and J_1^{c2} are observed, which indicate two second-order quantum phase transitions take place sequentially [28]. In order to determine J_1^{c1} and J_1^{c2} exactly, their scaling curves versus $1/\chi$ are plotted in the inset of Fig. 1. After polynomial fitting, we obtain $J_1^{c1} \simeq -0.32$ and $J_1^{c2} \simeq 0.062$ respectively.

Then, we calculate the ground-state bond energies. We find that, although the bond energies are continuous (see Fig. 2(a)), their first-order derivatives behave singularly at the same J_1^{c1} and J_1^{c2} as that determined by the bipartite entanglement (see Fig. 2(b)). According to the Feynman–Hellmann theorem ($\partial e/\partial\lambda = \langle\psi|\partial\hat{H}(\lambda)/\partial\lambda|\psi\rangle$, λ is a tunable parameter in the Hamiltonian), the first-order derivative of bond energy is similar to the second-order derivative of ground-state energy per site e [28]. The derivatives of bond energies become divergent at both critical points, which indicates the occurrence of two second-order QPTs. Considering that the bond energy consists of nearest-neighbor correlators ($\langle S_i^\sigma S_{i+1}^\sigma\rangle (\sigma = x, y,$ and $z)$), it is natural to speculate that the first-order derivative of the nearest-neighbor correlators should also exhibit similar characters. In Fig. 3(a), the nearest-neighbor correlation functions on odd bonds ($\langle S_{2i-1}^\sigma S_{2i}^\sigma\rangle$ ($\sigma = x, y,$ and z)) are provided. Although these curves themselves behave continuously, their first-order derivatives (see Fig. 3(b)) exhibit two singularities at J_1^{c1} and J_1^{c2}.

To uncover more information of the ground states,we calculate magnetization and order parameters. In Fig. 4,the curves of the Néel order parameter $M_{Neel}^z = \frac{1}{2}|\langle S_{2i-1}^z - S_{2i}^z\rangle|$ and the stripe order parameter $M_{stripe}^z = \frac{1}{4}|\langle S_{4n-3}^z + S_{4n-2}^z - S_{4n-1}^z - S_{4n}^z\rangle|$ are provided. From Fig. 4, the phase ($J_1 < J_1^{c1}$) with nonzero M_{Neel}^z should be a NP with configurations "$\cdots\uparrow\downarrow\uparrow\downarrow\cdots$" or "$\cdots\downarrow\uparrow\downarrow\uparrow\cdots$". While the phase in region $J_1 > J_1^{c2}$ with nonzero stripe order along the z-axis is verified to be an SP with spin configurations "$\cdots\uparrow\uparrow\downarrow\downarrow\cdots$" or "$\cdots\downarrow\downarrow\uparrow\uparrow\cdots$". The stripe phase was observed in 1D QCM by finite-size Lanczos exact diagonalization calculations [26] and confirmed subsequently by us [28]. We calculate the magnetization $M^\sigma = (1/N)\Sigma_{i=1}^N \langle S_i^\sigma\rangle$ $(\sigma = x, y, z)$, and find that it keeps zero in the whole parameter region. Then, we calculate the dimer order parameter [37] directly. We find that although the dimer order is very strong in the intermediate phase ($J_1^{c1} < J_1 < J_1^{c2}$), nonzero dimer order can also be observed in the other two phases. It means that three phases are all dimerized. Therefore, we would like to call this intermediate phase a disordered phase rather than a dimerized phase.