Quantum phase transition in the one-dimensional period-two and uniform compass model

Ke-Wei Sun,[1] Yu-Yu Zhang,[1] and Qing-Hu Chen[2,1,*]
[1]*Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China*
[2]*Center for Statistical and Theoretical Condensed Matter Physics, Zhejiang Normal University, Jinhua 321004, People's Republic of China*
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Quantum phase transitions in the one-dimensional period-two and uniform quantum compass model are studied by using the pseudospin transformation method and the trace map method. The exact solutions are presented, the fidelity, the nearest-neighbor pseudospin entanglement, spin and pseudospin-correlation functions are then calculated. At the critical point, the fidelity and its susceptibility change substantially, the gap of pseudospin concurrence is observed, which scales as $1/N$ (N is the system size). The spin-correlation functions show smooth behavior around the critical point. In the period-two chain, the pseudospin-correlation functions exhibit an oscillating behavior, which is absent in the uniform chain. The divergent correlation length at the critical point is demonstrated in the general trend for both cases.

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I. INTRODUCTION

Recently, the quantum compass model was introduced to describe some Mott insulators with orbit degeneracy by a pseudospin,[1,2] where the coupling along one of bonds is an Ising type, but different spin components are active along other bond directions. The disorder effect in this model was also examined.[3] The protected qubit is formed if it is separated from the low-energy excitations by a pseudospin excited gap. So a high quality factor, scalable and error-free scheme of quantum computation can be designed.[4] The symmetry of pseudospin Hamiltonians is usually much lower than SU(2),[5] and the result of numerical calculation has been shown that its eigenstates are at least twofold degenerate or highly degenerate and disordered.[6] The quantum *XX-ZZ* model, also called one-dimensional (1D) compass model, is constructed by antiferromagnetic order of X and Z pseudospin components on odd and even bonds, respectively.[7] In addition, the 1D quantum compass model is exactly the same as the 1D reduced Kitaev model.[8] The analytic eigenspectra in the latter model have been obtained, and it was shown that this model has one gapless phase. But the characters of the quantum phase transition have never been well studied previously. The realistic models of the orbital degeneracy are more complicated.

For the compass model, the pseudospins may lead to enhanced quantum fluctuations near the quantum phase transitions (QPTs) and to entangled spin-orbital ground states. The numerical results have indicated that a first-order QPT occurs at $J_x = J_z$ between two different states with spin ordering along either x or z directions.[6] Recently, the ground-state (GS) fidelity[9–15] and entanglement[16–24] emerged from quantum information science have been used in signaling the QPTs. To calculate these quantities accurately, it is necessary to know the exact GS wave function. The derivatives of the GS energy are intrinsically related to the GS fidelity,[13] both can be used to identify the QPTs. For the special case of two spin-1/2 system, the entanglement is given by the concurrence. Quantum entanglement is one of the most striking consequences of quantum correlation in many-body systems, shows a deep relation with the QPT.[16] Therefore understanding the entanglement is very important in QPTs.[17,18] In the context of QPTs, the quantum entanglement have been the subject of considerable interests in the Dicke model[19–21] and the *XY* model.[22,23]

On the other hand, experimental works on quasicrystals[25] and quasiperiodic superlattices[26] have inspired theoretical interests in 1D quasiperiodic systems. Period-two chain can be regarded as the intermediate one between uniform periodic chain and quasiperiodic chain, which have exhibited some unusual physical properties. In this work, we study the one-dimensional compass model for both uniform and period-two cases by using transfer-matrix method[24] and the method of Lieb *et al.*[27] The exact solutions for two cases are obtained. The GS fidelity and the energy gap between uniform and period-two quantum spin chain are calculated. The behaviors of the pseudospin correlations with periodic boundary condition are given.

The paper is organized as follows: In Sec. II, we give the model and the exact solution with periodic boundary condition. The calculation methods of fidelity and concurrence are introduced in Sec. III. The correlation functions are analyzed in Sec. IV. The paper is summarized in Sec. V, where we give some discussions and conclusions.

II. MODEL HAMILTONIAN AND EXACT SOLUTION

The Hamiltonian of one-dimensional compass model is given by

$$H = \sum_{i=1}^{N'} [J_i(\sigma_{2i-1}^z \sigma_{2i}^z + \beta \sigma_{2i}^x \sigma_{2i+1}^x)], \tag{1}$$

where J_i is the nearest-neighbor interaction, $\sigma_i^{x(z)}$ are the Pauli matrix on site i, $N = 2N'$ is the number of the sites, and β is the coupling parameter which determines the phase transition point. For $J_{2i} = J$ and $J_{2i+1} = \alpha J$, the model is a period-two case. By using the pseudospin (orbital) transformation method which is given by Brzezicki *et al.*,[7] we can define the modulated interactions for odd pairs of pseudospins $\{2i$

$-1,2i\}$ as $-\tau_i^z \equiv \sigma_{2i-1}^z \sigma_{2i}^z$, and the spin-flip operators of x direction are given by $\tau_i^x \equiv (-1)^{\sum_{k=1}^{i-1} s_k} \prod_{j=2i}^{2N'} \sigma_j^x$. The two neighboring odd bonds can be expressed as the even $\{2i,2i+1\}$ bonds by a product $-\tau_i^x \tau_{i+1}^x$. Then the Hamiltonian of one-dimensional compass model can be written as follows:

$$H_{\vec{s}} = -\sum_{i=1}^{N'-1} [J_i(\tau_i^z + \beta \tau_i^x \tau_{i+1}^x)] - J_{N'}[\tau_{N'}^z + (-1)^s \beta \tau_{N'}^x \tau_1^x]. \tag{2}$$

Note that it looks like but is different from the transverse field Ising model.

The vector $\vec{s}$ represents the state $(s_1, \cdots, s_{N'})$. Here $s_i = 1 (s_i = 0)$ labels that the two pseudospins of the odd bond $\{2i-1,2i\}$ are parallel (antiparallel). $s = \sum_{i=1}^{N'} s_i$ is the number of parallel odd pairs of spins. In this paper, we only discuss the ferromagnetic boundary condition of the quantum compass model, i.e., the case of the even s. The effective Hamiltonian (2) can be solved by using the Jordan-Wigner transformation for spin operators,

$$\tau_i^z = 1 - 2c_i^\dagger c_i, \tag{3}$$

$$\tau_i^x = (c_i + c_i^\dagger) \prod_{j<i} (1 - 2c_j^\dagger c_j), \tag{4}$$

where c_i and $c_i^\dagger$ are the anticommuting fermion operators. After this transformation, the effective Hamiltonian becomes

$$\begin{aligned} H_{\vec{s}} = &\sum_{i=1}^{N'-1} [2J_i c_i^\dagger c_i + J_i \beta (c_i c_{i+1}^\dagger - c_i^\dagger c_{i+1}^\dagger + c_i c_{i+1} - c_i^\dagger c_{i+1})] \\ &+ J_{N'} \beta (c_{N'} \tilde{c}_1^\dagger - c_{N'}^\dagger \tilde{c}_1^\dagger + c_{N'} \tilde{c}_1 - c_{N'}^\dagger \tilde{c}_1) + J_{N'} c_{N'}^\dagger c_{N'} \\ &- \sum_{i=1}^{N'} J_i, \end{aligned} \tag{5}$$

with

$$\tilde{c}_1 = c_1 (-1)^{1+s+\sum_{j=1}^{N'} c_j^\dagger c_j}. \tag{6}$$

Because we assume that the parity of s is even, it implies that only states with even numbers of Bogoliubov quasiparticles in the spectrum of the Hamiltonian (5). Under the periodic boundary condition ($c_{N'+1} = c_1$), the number of c fermions must be odd parity, as can easily be obtained from Eq. (6). Then the general form of the Hamiltonian is simplified to

$$\begin{aligned} H_{\vec{s}} = &\sum_{i=1}^{N'} [2J_i c_i^\dagger c_i + J_i \beta (c_i c_{i+1}^\dagger - c_i^\dagger c_{i+1}^\dagger + c_i c_{i+1} - c_i^\dagger c_{i+1})] \\ &- \sum_{i=1}^{N'} J_i. \end{aligned} \tag{7}$$

For the period-two case, we can rewrite Eq. (7) as the following form by neglecting the last constant term,

$$H = \sum_{i,j=1}^{N'} \left[c_i^\dagger A_{ij} c_j + \frac{1}{2}(c_i^\dagger B_{ij} c_j^\dagger + \text{H.c.}) \right], \tag{8}$$

where the nonzero elements of the matrices A and B are given by

$$A_{ij} = 2J_i \delta_{i,j} - J_i \beta \delta_{j,i+1} - J_j \beta \delta_{j,i-1},$$

$$B_{ij} = -J_i \beta \delta_{j,i+1} + J_j \beta \delta_{j,i-1};$$

$$A_{1N'} = A_{N'1} = -J_{N'} \beta,$$

$$B_{1N'} = -B_{N'1} = J_{N'} \beta.$$

Equation (8) can be diagonalized by using the Bogoliubov transformation,

$$\eta_k = \frac{1}{2} \sum_{i=1}^{N'} [(\phi_{ki} + \psi_{ki}) c_i + (\phi_{ki} - \psi_{ki}) c_i^\dagger],$$

$$\eta_k^\dagger = \frac{1}{2} \sum_{i=1}^{N'} [(\phi_{ki} + \psi_{ki}) c_i^\dagger + (\phi_{ki} - \psi_{ki}) c_i], \tag{9}$$

where ψ_{ki} is the eigenvector of the matrix $(\mathbf{A}+\mathbf{B})(\mathbf{A}-\mathbf{B})$ and ϕ_{ki} is that of the matrix $(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})$. The eigenvalues of both matrices are corresponding to Λ_k^2. We take $k = 0, \pm \frac{2\pi}{N'}, \pm 2\frac{2\pi}{N'}, \ldots, \pi$. This relation is satisfied with the periodic boundary condition. In general, the two eigenvectors (ϕ_{ki} and ψ_{ki}) satisfy the following equations:

$$(A-B)\vec{\psi}_k = \Lambda_k \vec{\phi}_k, (A+B)\vec{\phi}_k = \Lambda_k \vec{\psi}_k, \tag{10}$$

where $\vec{\phi}_k$ and $\vec{\psi}_k$ are two column vectors. The diagonalized result takes the form

$$H = \sum_k \Lambda_k \left(\eta_k^\dagger \eta_k - \frac{1}{2} \right). \tag{11}$$

The excitation energies $\Lambda_k \geq 0$. At zero temperature, the QPT points are those parameters that satisfy the condition $\Lambda_k = 0$, and the two coupled coefficients of the Bogoliubov transformation satisfy the following equations:

$$\Lambda_k \phi_{k,i} = 2J_i \psi_{k,i} - 2J_{i-1} \beta \psi_{k,i-1},$$

$$\Lambda_k \psi_{k,i} = 2J_i \beta \phi_{k,i} - 2J_i \beta \phi_{k,i+1}, \tag{12}$$

which can be derived from Eq. (10). For the period-two case, i.e., $J_{2i} = J$ and $J_{2i+1} = J\alpha$, if we take $J=1$ and assume that $\psi_{k,2n} = A e^{i2nk}$ and $\psi_{k,2n+1} = B e^{i(2n+1)k}$, the exact results of Λ_k can be obtained analytically from the coupled Eq. (12) by using the trace map method. The result is expressed as

$$\begin{aligned} \Lambda_{k\pm}^2 = &\pm \sqrt{4J^4(\beta^2+1)^2(\alpha^2-1)^2 + 64\alpha^2 J^4 \beta^2 \cos^2 k} \\ &+ (\alpha^2+1)(2J^2\beta^2 + 2J^2). \end{aligned} \tag{13}$$

The excitation energies have two branches (Λ_{k-} and Λ_{k+}). For a special case $\alpha=1$, i.e., the uniform periodic chain, the excitation energies can be simplified as $2J\sqrt{1+\beta^2-2\beta \cos k}$,

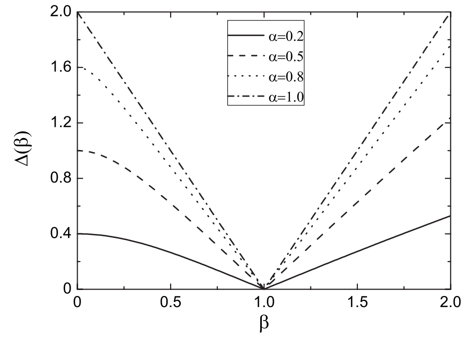

FIG. 1. Pseudospin excitation gap Δ on uniform and period-two cases of the compass model. The gaps collapse at the quantum phase-transition point at $\beta=1$ for different values of α.

which is the same as that in Ref. 7. The QPT point is determined by Λ_{k-}. At the critical point, the equation can be decoupled for $\Lambda_k=0$. One of Eq. (12) is rewritten as $\phi_{k,i+1} = \frac{1}{\beta}\phi_{k,i}$. Due to the periodic boundary condition, $(\frac{1}{\beta})^{N'}=1$ should be satisfied. The only possibility is $\beta=1$, i.e., there is only one QPT point at $\beta=1$ in this case. On the other hand, the GS energy is expressed as $E_0=-\frac{1}{2}\Sigma_k\Lambda_k$ which includes the spectra of the $\pm$ branches. In thermodynamic limit, the summation can be replaced by an integral,

$$E_0 = -JN'\frac{1}{2\pi}\int_0^{\pi}(\Lambda_{k-}+\Lambda_{k+})dk. \tag{14}$$

The pseudospin excitation gap Δ, which is energy difference between the first-excited state and the ground state, is equal to Λ_{0-}, which disappears at $\beta=1$.

From the Fig. 1, we can find that the symmetries of the pseudospin gaps are broken more obviously as β is away from the QPT point in the period-two model. The symmetries remain for the uniform model. The quantum critical point is fixed at $\beta_c=1$ which separates the disorder phase. In the vicinity of the quantum critical point, the linear relation $\Delta=\sqrt{10(\alpha^2+1)-2\sqrt{25\alpha^4+14\alpha^2+25}}|1-\beta|$ is generally satisfied.

III. FIDELITY AND PSEUDOSPIN CONCURRENCE

The exact GS wave function of the system must be obtained in order to calculate the fidelity and concurrence. Similar to the Bardeen, Cooper, and Schrieffer GS wave function, we can write the present GS wave function as[28]

$$|\Psi_0(\beta)\rangle = \prod_k \eta_k|Vac\rangle \quad \text{for all } k. \tag{15}$$

According to Eq. (9) and the definition of the fidelity[11]

$$F(\beta,\delta) = |\langle\Psi_0(\beta)|\Psi_0(\beta+\delta)\rangle|, \tag{16}$$

where δ is a small quantity ($\delta=10^{-4}$ is taken in our calculation), the fidelity and its susceptibility can be given by

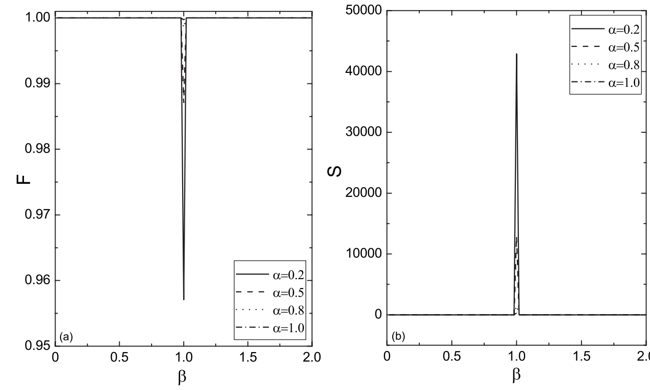

FIG. 2. The fidelity and the susceptibility of the period-two compass model versus β for $\alpha=0.2,0.5,0.8,1.0$ and $N'=100$. The first QPT point is obviously found at $\beta_c=1$.

$$F(\beta,\delta) = \prod_k \left|\sum_i \frac{1}{4}[\phi_{ki}(\beta)-\psi_{ki}(\beta)] \times[\phi_{ki}(\beta+\delta)-\psi_{ki}(\beta+\delta)]\right|, \tag{17}$$

$$S(\beta) = 2\lim_{\delta\to 0}\frac{1-F(\beta,\delta)}{\delta^2}. \tag{18}$$

The numerical results for the GS fidelity and its susceptibility are plotted in Fig. 2. An abrupt jump occurs in the vicinity of the QPT point ($\beta_c=1$) as a consequence of the dramatic change of the structure of the GS. It agrees exactly with our analytical derivations. One can see level crossing at $\beta=\beta_c$, indicating the first-order QPT in this model.

In recent years, the concept of concurrence is usually adopted as the measure of the entanglement in spin-1/2 systems. We will give the nearest-neighbor pseudospin two-point correlation functions to calculate the nearest-neighbor concurrence (NNC) of the system. Because of the reflection symmetry, the global phase flip symmetry, and the Hamiltonian being real, the nonzero elements are given by[18,27]

$$\langle\tau_i^x\tau_{i+1}^x\rangle = G_{i,i+1}, \langle\tau_i^y\tau_{i+1}^y\rangle = G_{i+1,i},$$

$$\langle\tau_i^z\tau_{i+1}^z\rangle = G_{i,i}G_{i+1,i+1} - G_{i,i+1}G_{i+1,i},$$

$$\langle\tau_i^z\rangle = -G_{i,i}, \tag{19}$$

where $G_{i,j}=-\Sigma_k\psi_{ki}\phi_{kj}$. The definition of concurrence is given by $C(i,j)=\max[r_1(i,j)-r_2(i,j)-r_3(i,j)-r_4(i,j),0]$, where $r_\alpha(i,j)$ are the square roots of the eigenvalues of the product matrix $R=\rho_{ij}\tilde{\rho}_{ij}$ in descending order. The spin flipped matrix $\tilde{\rho}_{ij}$ is defined as $\tilde{\rho}_{ij}=(\sigma^y\otimes\sigma^y)\rho_{ij}^*(\sigma^y\otimes\sigma^y)$. The ρ_{ij} is the density matrix for a pair of qubits from a multiqubit state. In this way, we can calculate the NNC of pseudospins. For the period-two chain, the concurrence $C_{2i,2i+1}$ and $C_{2i+1,2i+2}$ are different. So we use the average concurrence $C = \frac{1}{2}(C_{2i,2i+1}+C_{2i+1,2i+2})$.

The numerical results for the concurrence as a function of β are given in Fig. 3. It is shown that the maximum value of

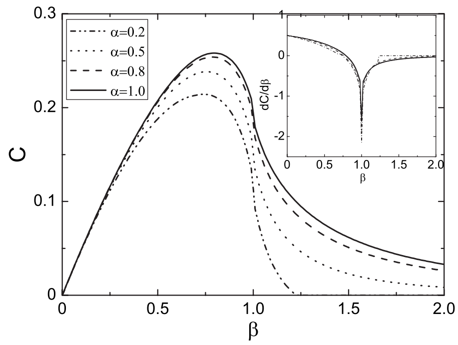

FIG. 3. The concurrence C versus β for $\alpha=0.2,0.5,0.8,1.0$ ($N'=100$). The inset shows the derivative $\partial_\beta C$ as a function of β.

the concurrence gradually increases with the increase of parameter α. If α is small enough, the entanglement of nearest-neighbor pseudospins disappears in the larger β regime. A cusp of the first derivative of the concurrence occurs at the critical point $\beta=1$, similar to those in Ref. 16.

A gap is found in the curve of NNC versus β at the QPT point β_c in our calculation of the pseudospin concurrence. If the pseudospin chain goes to infinite, the gap has the critical behavior with $\Delta C \propto N^{-1}$, as shown in the inset of Fig. 4. Obviously, it is the finite-size effect. The question then arises: what is the origin of the concurrence gap? The answer is the symmetry of system which has been assumed by the ferromagnetic even-pseudospin chains with periodic boundary condition in this paper. The QPT in the 1D compass model is of first order,[4,7] the scaling behaviors at the critical point should be absent. But the discontinuousness of the concurrence at the QTP may exhibit the finite-size scaling behavior $N\rightarrow -1$,[29] consistent with the present observation. Due to the concurrence gap, the value of $\partial_\beta C$ becomes minimum at the critical point. However, the maximum value of the concurrence occurs below β_c is not related to the critical point. The present results for the concurrence are similar to those in the periodic quantum Ising chain model.[18]

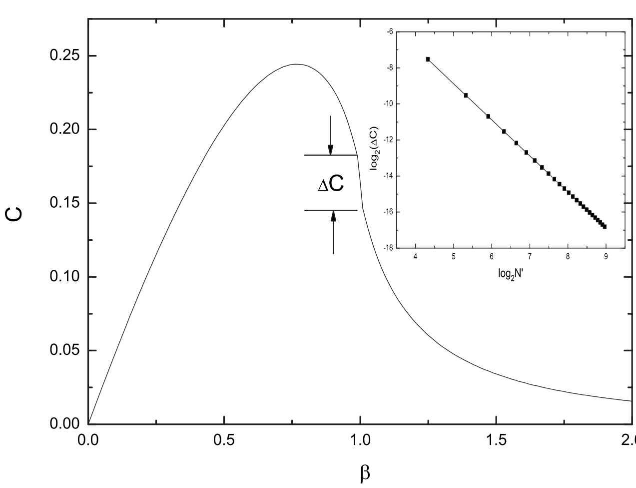

FIG. 4. The NNC as a function of β with $\alpha=0.6$ for $N'=100$. A gap ΔC for the concurrence is found at the critical point. The inset shows the size scaling of the gap.

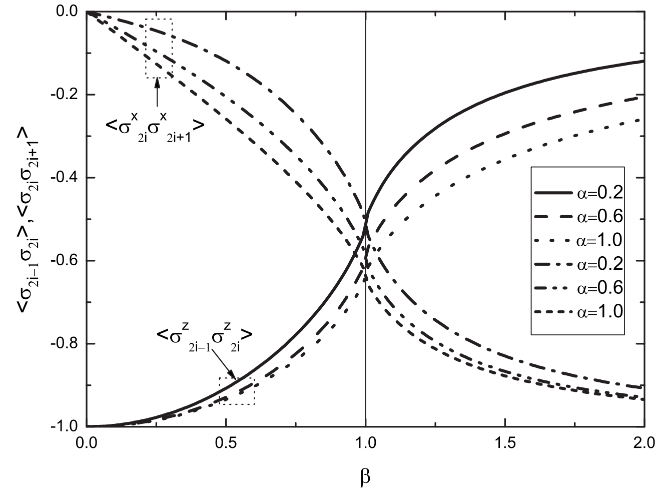

FIG. 5. Spin-correlation functions in the period-two chain and uniform chain for $\alpha=0.2,0.6,1.0$ and $N'=100$.

IV. SPIN AND PSEUDOSPIN-CORRELATION FUNCTIONS

First, we show the numerical results of the ground-state spin correlations on odd $\{2i-1,2i\}$ and even $\{2i,2i+1\}$ bonds as a function of β with a periodic boundary condition. The value of $\langle\sigma^z_{2i-1}\sigma^z_{2i}\rangle$ gradually increases with β while $\langle\sigma^x_{2i}\sigma^x_{2i+1}\rangle$ decreases with β, as shown in Fig. 5. The crossing points of $\langle\sigma^z_{2i-1}\sigma^z_{2i}\rangle$ and $\langle\sigma^x_{2i}\sigma^x_{2i+1}\rangle$ curves for the same α occur at the quantum critical point. Actually, the compass model is a kind of pseudospin Ising chains at $\beta=0$ and $\beta\rightarrow\infty$. As a result, the curves of spin correlations versus β are asymmetric. So $\langle\sigma^z_{2i-1}\sigma^z_{2i}\rangle\rightarrow 0$ and $\langle\sigma^x_{2i}\sigma^x_{2i+1}\rangle\rightarrow -1$ as $\beta\rightarrow\infty$.

It is found that the correlation gradually increases with the decreasing α. When $\alpha=1$, the numerical result at the critical point is the same as the analytical result by Brzezicki *et al.*[7]

Finally, we calculate the distance dependence of the pseudospin correlator $\langle\tau^x_i\tau^x_{i+r}\rangle$ under the periodic boundary condition for the period-two and uniform cases. The two-point correlation function is given by[27]

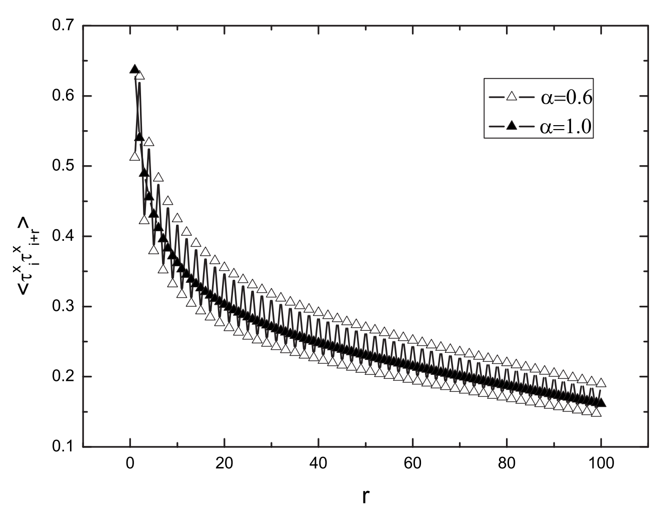

FIG. 6. Distance dependence of $\langle\tau^x_i\tau^x_{i+r}\rangle$ correlator at the critical point. The parameters are $\alpha=0.6,1.0$ and $N'=200$.

$$\langle \tau_i^x \tau_{i+r}^x \rangle = \begin{vmatrix} G_{i,i+1} & G_{i,i+2} & \cdots & G_{i,i+r} \\ G_{i+1,i+1} & G_{i+1,i+2} & \cdots & G_{i+1,i+r} \\ \cdots & \cdots & \cdots & \cdots \\ G_{i+r-1,i+1} & G_{i+r-1,i+2} & \cdots & G_{i+r-1,i+r} \end{vmatrix}, \quad (20)$$

which has the form of Toeplitz determinant. When $r \to \infty$, the correlators gradually decrease and approach the asymptotic value for large r in an algebraic way.[7] This correlator is positive for all r, indicating that there is the long-range ferromagnetic order. It is interesting to find that the oscillation occurs for $\alpha \neq 1$, i.e., for period-two chain, which can be attributed to the different coupling coefficients of odd and even bonds. However, the similar trend appears in both cases, as shown in Fig. 6.

V. SUMMARY AND DISCUSSION

By using the pseudospin transformation method and the trace map method, we obtain the exact solution of one-dimensional compass model with periodic boundary condition. The parameter α determines the symmetries of finite pseudospin excitation gap Δ, but the phase transition point is still fixed at $\beta = 1$. The quantum critical point separates the disorder phase. The pseudospin liquid disordered ground state is the universal features in the 1D compass model. The numerical methods to calculate the fidelity and concurrence are also given. We observe a first-order quantum phase transition between two different disordered phases. The concurrence gap ΔC displays the scaling property $N = -1$. The spin and pseudospin-correlation functions are calculated. Curves for the two spin-correlation function cross exactly at the critical point for any value of α. It is observed that the distance dependence of $\langle \tau_i^x \tau_{i+r}^x \rangle$ correlator displays oscillation in the period-two case, and a divergent correlation length at the critical point is observed in both uniform and period-two chains.

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*Corresponding author; qhchen@zju.edu.cn

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