Letter

Order by disorder in frustration-free systems: Quantum Monte Carlo study of a two-dimensional PXP model

Mingxi Yue,[1,*] Zijian Wang,[1,2,*] Bhaskar Mukherjee,[1,3] and Zi Cai[1,4,5,†]

[1]*Wilczek Quantum Center, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China*

[2]*Zhiyuan College, Shanghai Jiao Tong University, Shanghai 200240, China*

[3]*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA*

[4]*Key Laboratory of Artificial Structures and Quantum Control, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China*

[5]*Shanghai Research Center for Quantum Sciences, Shanghai 201315, China*

(Received 1 April 2021; revised 4 May 2021; accepted 6 May 2021; published 18 May 2021)

In this study, an order-by-disorder mechanism has been proposed in a two-dimensional PXP model, where the extensive degeneracy of the classical ground-state manifold is due to strict occupation constraints instead of geometrical frustrations. By performing an unbias large-scale quantum Monte Carlo simulation, we find that local quantum fluctuations, which usually work against long-range ordering, lift the macroscopic classical degeneracy and give rise to a compressible ground state with charge-density-wave long-range order. A simple trial wave function has been proposed to capture the essence of the ground-state of the two-dimensional PXP model. The finite-temperature properties of this model have also been studied, and we find a thermal phase transition with a universality class of a two-dimensional Ising model.

DOI: 10.1103/PhysRevB.103.L201113

Introduction. The order-by-disorder mechanism is one of the most remarkable phenomena in geometrically frustrated materials, where it is impossible to simultaneously minimize the interacting energy for all bonds in the system. Hence extensive degeneracy arises in the classical ground-state manifold. Such a classical ground-state degeneracy may be partially or completely lifted by subtle effects that normally work against ordering in a process termed "order by disorder," where particular configurations are selected out of the degenerate manifold, and long-range order is restored [1–3]. For instance, thermal fluctuations can give rise to entropic differences between configurations, hence degeneracy-breaking free-energy terms at finite temperature [1,2], while at zero temperature taking into account quantum fluctuations may lead to degeneracy-breaking zero-point energy that favors ordered states [3,4]. Up to now, most studies in this field have concentrated on frustrated systems. A question thus arises: Is frustration a necessity for us to observe the order-by-disorder phenomenon?

In this paper, we attempt to answer this question, focusing for simplicity on a two-dimensional (2D) PXP model on a square lattice. In spite of its extreme simplicity, this model not only provides a prototypical example of the order-by-disorder phenomenon in a frustration-free system, but it is also closely related to recent progress with quantum simulators based on Rydberg atomic systems [5–7], where a neutral atom can strongly interact with its neighbors via a Rydberg blockade mechanism, which prevents two nearby atoms from being simultaneously excited into the excited states [8]. In such a highly tunable and controllable platform, the interplay between constraints resulting from the Rydberg blockade and the quantum fluctuations could give rise to exotic quantum matter [9–13] as well as nonequilibrium quantum many-body dynamics [14–17].

By performing a numerically exact quantum Monte Carlo (QMC) simulation [18], we study the ground state of a PXP model in a square lattice, which can be realized in an interacting Rydberg atomic system with zero detuning [19]. It is shown that in the absence of laser driving, any classical configuration satisfying the Rydberg blockade condition is a ground state of this model, yielding a macroscopic degeneracy in the ground-state manifold. For each atom in the lattice, the driving laser field induces coupling between the ground state and the Rydberg state, thus it acts as a local quantum fluctuation. Counterintuitively, such an off-diagonal term (in the Fock basis), which usually works against long-range ordering, is found to lift the macroscopic classical degeneracy and give rise to a charge-density-wave state with a spontaneous Z_2 symmetry breaking. This result has provided a different perspective on the order-by-disorder phenomenon, where the extensive degeneracy lifted by quantum fluctuations comes from occupation constraints instead of geometrical frustration.

Model and method. In terms of the hard-core boson language, the Hamiltonian of a PXP model reads

$$H = \Omega \sum_{\mathbf{i}} (\tilde{b}_{\mathbf{i}} + \tilde{b}_{\mathbf{i}}^{\dagger}), \tag{1}$$

where $\tilde{b}_{\mathbf{i}}$ ($\tilde{b}_{\mathbf{i}}^{\dagger}$) is the annihilation (creation) operator of the hard-core bosons operating on the constraint Hilbert space $\mathbb{H}$ that excludes those configurations with two bosons located on neighboring sites. Similar models have also been proposed to

*These authors contributed equally to this work.

†zcai@sjtu.edu.cn

describe correlated bosonic systems in a tilted optical lattice [20–22]. In terms of spin-$\frac{1}{2}$ operators, Eq. (1) describes a PXP model with the Hamiltonian $H_{\rm PXP} = \Omega \sum_{\mathbf{i}} \tilde{\sigma}_{\mathbf{i}}^{x}$. Compared to the one-dimensional version of the related models, whose ground state and nonequilibrium properties have been intensively studied [16,17,23–26], the 2D PXP model has been much less studied [27,28].

The PXP model can also be realized in a strongly interacting Rydberg atomic system subjected to a coherent laser driving field, whose Hamiltonian reads as follows:

$$H_R = \sum_{\mathbf{i}} [\Omega(|g\rangle_{\mathbf{i}}\langle e| + |e\rangle_{\mathbf{i}}\langle g|) - \delta|e\rangle_{\mathbf{i}}\langle e|] + V \sum_{\langle \mathbf{ij}\rangle} \hat{n}_{\mathbf{i}}^{e}\hat{n}_{\mathbf{j}}^{e}, \quad (2)$$

where $\langle \mathbf{ij}\rangle$ indicates a pair of adjacent lattice sites in the $L \times L$ square lattice. $|g\rangle_i$ ($|e\rangle_i$) denote the internal atomic ground (excited) state of the atom on site $\mathbf{i}$, and $\hat{n}_{\mathbf{i}}^{e} = |e\rangle_{\mathbf{i}}\langle e|$ is the density operator of the excited state on site $\mathbf{i}$. Ω and δ are the Rabi frequency and the detuning of the coherent laser driving field, and V is the strength of the interaction between the Rydberg atoms. Here we only consider the nearest-neighbor interaction, which can be experimentally realized by properly tuning the Rydberg blockade radius. The ground-state phase diagram of Eq. (2) has been studied using the density matrix renormalization group (DMRG) method, where different crystalline ground states and corresponding quantum phase transitions have been found [13]. Here, to illustrate its relationship with the order-by-disorder phenomena, we consider Eq. (2) in the limit $V \to \infty$ and $\delta \to 0$, where Eq. (2) turns into the 2D PXP model (1).

Throughout this paper, we study the 2D PXP model described by Eq. (1) using a continuous-time QMC algorithm, which allows us to study both the ground state and thermal properties up to a significantly large system size. Notice that local quantum fluctuation in Eq. (1) does not result in a sign problem in the Monte Carlo sampling, nor does the occupation constraint, thus the QMC simulation is unbiased and numerically exact. To sample those (imaginary) time-space configurations according to their weights in the partition function, we choose an ergodic set of updates consisting of randomly inserting/removing on-site pair vertices in the configurations [29]. The constraint complicates the simulation by introducing correlations between adjacent sites. To approach the ground state in the QMC simulations, we scale the inverse temperature as $\beta = L$ and take the thermodynamic limit $L \to \infty$.

Classical limit. We first focus on the case without quantum fluctuations ($\Omega = 0$), where any classical configuration in the Fock basis satisfying the occupation constraint has the same energy $E = 0$. In a 1D lattice, the number of these states diverges exponentially with the system size L as $\sim e^{L\ln\alpha}$ with $\alpha = (\sqrt{5}+1)/2$ [30]. In a 2D square lattice, the dimension of this constraint Hilbert space $\mathbb{H}$ still diverges exponentially with the number of lattice sites $N = L^2$, while it is difficult to find an analytical expression as simple as that in the 1D case.

Order by disorder in the ground state. Now we consider the effect of the local quantum fluctuation in Eq. (1), which breaks the particle number conservation. We first focus on the ground-state properties. The finite-size scaling of the charge-density-wave (CDW) order parameter

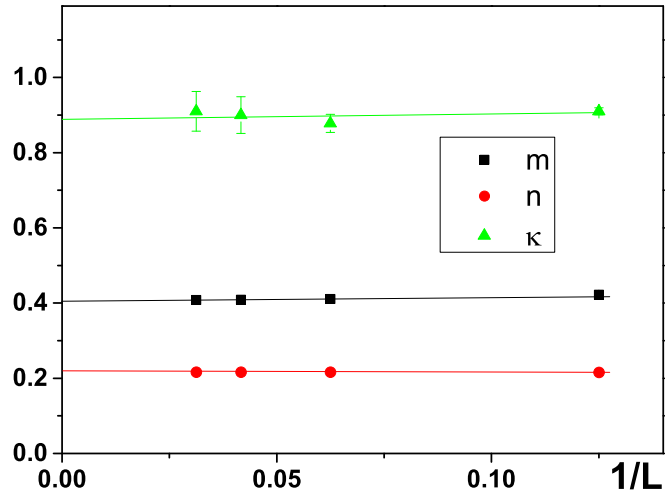

FIG. 1. Finite-size scaling of the CDW order parameter m, density of the bosons n, and the compressibility κ in the 2D $L \times L$ PXP model obtained by QMC simulations with $\beta = L$.

$$m = \frac{2}{N}\sqrt{\left\langle \left[\sum_{\mathbf{i}} (-1)^{i_x+i_y}\hat{n}_{\mathbf{i}}\right]^2\right\rangle} \quad (3)$$

as well as the density of the bosons

$$n = \frac{1}{N}\sum_{\mathbf{i}}\langle n_{\mathbf{i}}\rangle \quad (4)$$

are plotted in Fig. 1, from which we can find a nonvanishing CDW order parameter $m_0 = 0.403(6)$ at the density $n_0 = 0.221(5)$ in the thermodynamic limit. These results indicate that the local quantum fluctuation, which usually works against long-range ordering, selects a quantum state with CDW long-range order from the extensively degenerate classical ground-state manifold. Notice that the physical quantities of this model barely depend on the system size L, which indicates a feature of locality. In other words, the ground state might be close to a product state. More information on the ground state can be obtained from the compressibility, which is defined based on the fluctuations of total particle numbers as

$$\kappa = \frac{\beta}{L^2}(\langle \hat{N}^2\rangle - \langle \hat{N}\rangle^2), \quad (5)$$

where $\hat{N} = \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}}$ is the total particle number operator of the hard-core bosons. The finite-size scaling of κ is also plotted in Fig. 1, which indicates that the ground state is compressible. However, due to the explicit breaking of the U(1) symmetry in Eq. (1), its ground state is not a superfluid.

The order-by-disorder phenomenon in this frustration-free system and emergent CDW order can be understood as a consequence of the competition between the quantum fluctuations and the occupation constraint. The quantum fluctuations (spin-flip terms $\tilde{\sigma}_i^x$ in spin-$\frac{1}{2}$ language) could further lower the energy of the system by resonating the degenerate classical configurations, thus they are energetically favored in the ground state. However, two "spin-flip" operators acting

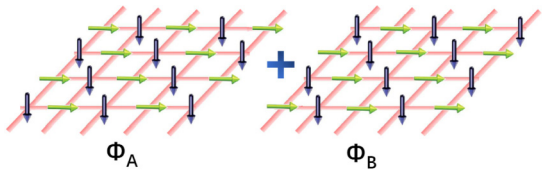

FIG. 2. Schematic diagram of the trial wave function in Eq. (6) in terms of spin language.

on a pair of adjacent sites will inevitably give rise to the configurations that violate the occupation constraint. As a compromise, the system favors a ground state with as many "spin-flips" as possible, while they try to keep away from each other to avoid a Rydberg blockade. One of the simplest examples satisfying these requirements is a product state with a wave function: $\Phi_A = \prod_i |\phi\rangle_i$, where $|\phi\rangle_i = |0\rangle_i$ if $i \in A$, and $|\phi\rangle_i = \frac{1}{\sqrt{2}}(|0\rangle_i - |1\rangle_i)$ if $i \in B$, with A (B) indicating the A (B) sublattice in the square lattice. $|0\rangle_i$ ($|1\rangle_i$) indicates the ground (excited) state of the Rydberg atoms on site i. The state Φ_A as well as its sublattice symmetric counterpart $\Phi_B = \Phi_{A\to B}$ spontaneously break the translational symmetry, thus it exhibits long-range order, which can qualitatively explain the observed CDW order in the ground state of Eq. (1).

Since there is no spontaneous symmetry breaking for any finite system, we propose a trial wave function

$$\Phi_{\text{trial}} = \frac{1}{\sqrt{2}}(\Phi_A + \Phi_B), \tag{6}$$

which is an equally weighted superposition of the symmetry-breaking states to restore the symmetry but keep the long-range CDW correlations. In the Fock basis, the wave function Φ_A (Φ_B) indicates an equally weighted superposition of all the possible classical configurations in sublattice A (B), while it leaves the other sublattice empty. A similar trial wave function without translational symmetry breaking has been proposed for the 1D PXP model [31] (see Fig. 2).

Such a trial wave function in Eq. (6), in spite of its extreme simplicity, can qualitatively capture most features of the ground state of Eq. (1). To verify this point numerically, we compare the results predicted by this trial wave function to our numerical results (see Table I). We first focus on the physical quantities. For instance, the average energy predicted by the trial wave function (6) is -0.5Ω, which is only 2.4% higher than its exact value.an In addition, the particle density predicted by wave function (6) is 0.25, which is also not very far from its exact value 0.22. To directly compare the trial wave function to the exact one, we perform exact diagonalization to

TABLE I. Comparisons of physical quantities (particle density n, CDW order parameter m, and average energy $e_g = E_g/N$) of the ground state obtained by the trial wave function, the Lanczos method for a 6×6 system, and the QMC simulations.

	n	m	e_g
trial	0.25	0.5	-0.5Ω
Lanczos (6×6)	0.209	0.417	-0.513Ω
QMC ($L \to \infty$)	0.221	0.403	-0.512Ω

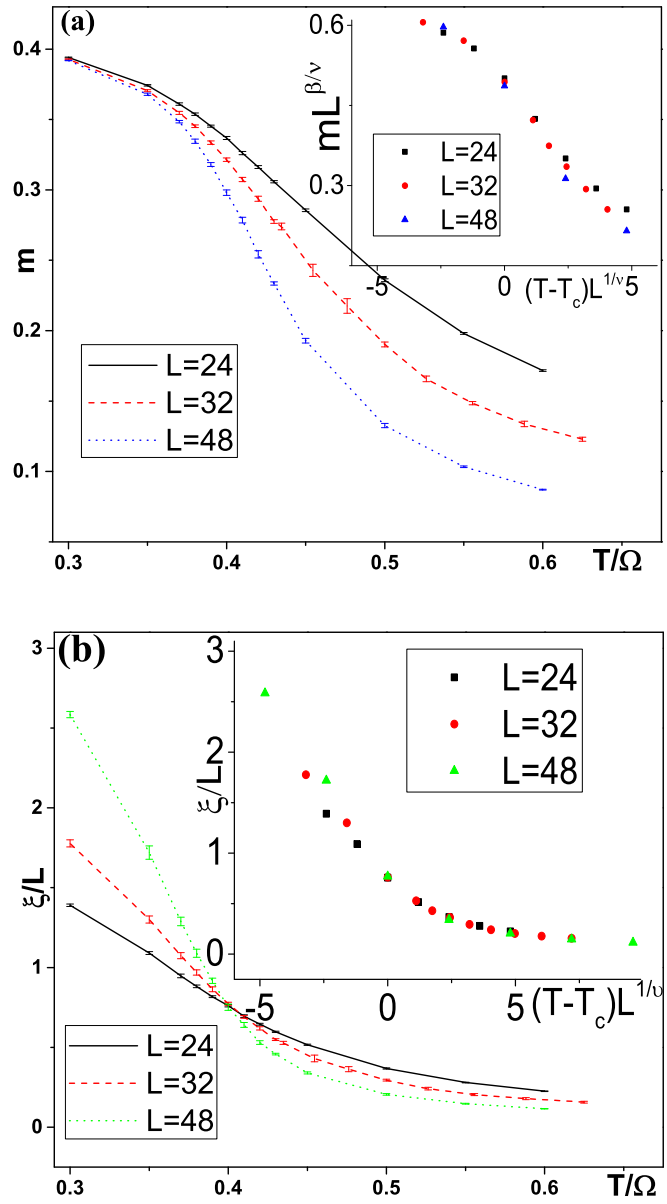

FIG. 3. (a) CDW order parameter m and (b) renormalized correlation length ξ/L as a function of temperature T for a different system size L in the QMC simulation. The insets are the data collapse for (a) the order parameter and (b) the renormalized correlation length using the critical exponents $\nu = 1$ and $\beta = 1/8$.

obtain the exact ground-state wave function $|\Phi_E\rangle$. Notice that the occupation constraint significantly reduces the dimension of the Hamiltonian matrix, thus enabling us to obtain $|\Phi_E\rangle$ by the Lanczos algorithm for a small system. Take a 6×6 system for example. The dimension of the constraint Hilbert space $\mathbb{H}$ is only 0.0035% of that of the full Hilbert space, and the overlap between the exact wave function and the trial wave function (6) is $\langle\Phi_{\text{trial}}|\Phi_E\rangle = 0.848\,88$, which is pretty high considering that the dimension of these two wave functions is 2 406 862, and there are no tunable parameters in the trial wave function (6).

Finite-temperature phase transition. It has been shown that the ground state of the 2D PXP Eq. (1) spontaneously breaks

Z_2 translational symmetry and exhibits CDW long-range order. Considering the fact that there is only one parameters Ω in PXP Eq. (1), at zero temperature, this CDW order will persist irrespective of the strength of the quantum fluctuation Ω. At finite temperature, one may expect a competition between quantum and thermal fluctuations, which may result in a finite-temperature phase transition. To verify this point numerically, we calculate the CDW order parameter as a function of temperature, as shown in Fig. 3(a). We also calculate the CDW correlation length ξ (along the x-direction) in the QMC simulation as [32]

$$\xi = \frac{1}{q_1}\sqrt{\frac{S(\pi,\pi)}{S(\pi+q_1,\pi)}-1}, \tag{7}$$

where $S(\mathbf{Q}) = \frac{1}{N^2}\sum_{ij} e^{i\mathbf{Q}\cdot(\mathbf{i}-\mathbf{j})}\langle n_\mathbf{i} n_\mathbf{j}\rangle$ is the structure factor of the density-density correlation, $q_1 = \frac{2\pi}{L}$. The CDW order parameter m is defined the same as Eq. (3). The normalized correlation length ξ/L as a function of temperature for systems with different sizes L has been plotted in Fig. 3(b), from which we can find a scaling invariant point indicating a critical point at $T_c = 0.4\Omega$. Near the critical point, the correlation length diverges as $\xi \sim |T - T_c|^{-\nu}$, and the order parameter scales as $m \sim |T - T_c|^{\beta}$. To explore the universal class of this phase transition, we study the scaling behavior around the critical point. The data collapses as shown in the insets of Fig. 3 indicate that the critical exponents $\beta = 1/8$ and $\nu = 1$, which agrees with those of the 2D Ising universal class.

Conclusion and outlook. In summary, we observed an order-by-disorder phenomenon in a frustration-free system, where the extensive classical ground-state degeneracy is due to an occupation constraint instead of geometrical frustration. It is shown that in a 2D PXP model, the competition between local quantum fluctuation and an occupation constraint gives rise to a compressible ground state with CDW long-range order, which could be destroyed by thermal fluctuation via a finite-temperature phase transition with a universality class of a 2D Ising model.

Future developments will include a generalization of our method and result to systems with different types of CDW orders and quantum fluctuations. For instance, Samajdar *et al.* have proposed complex CDW orders in 2D interacting Rydberg atomic systems [13]. Even though most of them are due to the direct interactions between the Rydberg atoms in the classical limit, there could be some regimes in the global phase diagram whose CDW orders are induced by the order-by-disorder mechanism. Different types of quantum fluctuations, especially those preserving the total particle number ($\tilde{b}_i^\dagger \tilde{b}_j$, for instance), are of particular interest, and one may expect a CDW-to-superfluid transition with increasing doping in this case. In addition, the ground-state phase diagram of the PXP models with additional terms (e.g., the chemical potential $-\mu\tilde{n}_i$) and the corresponding quantum critical behavior can also be studied [13], even though this term with $\mu \neq 0$ lifts the extensive degeneracy of the corresponding classical model ($\Omega = 0$), thus it is not directly related to the order-by-disorder phenomenon discussed here. Furthermore, our QMC algorithm is ready to be generalized to frustrated systems (e.g., kagome and triangle lattices), where the interplay between the frustration, quantum fluctuations, and constraint may give rise to exotic quantum many-body states [33,34].

Acknowledgments. This work is supported by the National Key Research and Development Program of China (Grants No. 2020YFA0309000 and No. 2016YFA0302001), NSFC of China (Grant No. 11574200), and Shanghai Municipal Science and Technology Major Project (Grant No. 2019SHZDZX01).

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