Stripes and spin-density waves in the doped two-dimensional Hubbard model: ground state phase diagram

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We determine the spin and charge orders in the ground state of the doped two-dimensional (2D) Hubbard model in its simplest form, namely with only nearest-neighbor hopping and on-site repulsion. At half-filling, the ground state is known to be an anti-ferromagnetic Mott insulator. Doping Mott insulators is believed to be relevant to the superconductivity observed in cuprates. A variety of candidates have been proposed for the ground state of the doped 2D Hubbard model. A recent work employing a combination of several state-of-the-art numerical many-body methods established the stripe order as the ground state near 1/8 doping at strong interactions. In this work, we apply one of these methods, the cutting-edge constrained-path auxiliary field quantum Monte Carlo (AFQMC) method with self-consistently optimized gauge constraints, to systematically study the model as a function of doping and interaction strength. With careful finite size scaling based on large-scale computations, we map out the ground state phase diagram in terms of its spin and charge order. We find that modulated antiferromagnetic order persists from near half-filling to about 1/5 doping. At lower interaction strengths or larger doping, these ordered states are best described as spin-density waves, with essentially delocalized holes and modest oscillations in charge correlations. When the charge correlations are stronger (large interaction or small doping), they are best described as stripe states, with the holes more localized near the node in the antiferromagnetic spin order. In both cases, we find that the wavelength in the charge correlations is consistent with so-called filled stripes.

I. INTRODUCTION

The Hubbard model is one of the most studied quantum many-body systems in condensed matter physics. With a very simple form, it plays a crucial role in the exploration of correlation effects in electronic systems. It is a “paradigmatic” model in the realm of condensed matter physics, like the Ising model in statistical physics. The Hubbard model hosts rich physics with the variation of interaction strength, doping level, temperature, and lattice geometry. On a square lattice, the doped Hubbard model is widely believed to be relevant to high-Tc superconductivity in cuprates. Despite the formal simplicity of the Hamiltonian, the Hubbard model cannot be solved analytically, except for a few special cases in the parameter space. Numerical methods play a key role in the study of the Hubbard model.

At half-filling, it is now established that the Hubbard model has an anti-ferromagnetic Mott insulating ground state for any finite value of the interaction strength. What happens when holes are added to the anti-ferromagnetic state may have a crucial role to understanding the mechanism of high-Tc superconductors. Previously, a variety of ground state candidates were obtained with different methods, including stripe order/spin density waves and superconductivity. A study in 2017 involving four state-of-the-art numerical many-body methods concluded that, near 1/8 doping, a filled (i.e., with wavelength equal to inverse doping) stripe state was the ground state. More evidence since then, from other numerical methods studying systems with sizes sufficient to accommodate the wavelength of the stripe state, has confirmed the existence of stripe order in the doped Hubbard model.

The study of stripe order in the Hubbard model can be traced back to 1980s in Hartree-Fock and 1990s in density matrix renormalization group (DMRG) calculations. Work to study stripes in cuprate superconductors was also performed on the two-dimensional Hubbard model using dynamical mean-field theory and slave boson methods. Constrained-path auxiliary-field quantum Monte Carlo (AFQMC) calculations showed spin-density wave states at intermediate interaction strengths which turned into stripe states with increasing interaction, and determined the wavelength of the collective modes. In both the SDW and stripe states, a unidirectional order is established with the anti-ferromagnetic correlations displaying a π phase flip across nodes. In the SDW state, the hole density variation is small. In the stripe phase, the doped holes concentrate in the nodal region of the spin modulation.

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II. MODEL AND METHODOLOGY

A. Model

The Hamiltonian of the Hubbard model is as follows:

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i v_{i\sigma} n_{i\sigma} \] (1)

where the coordinates of the lattice site labeled \( i \) are given by \( r_i = (i_x, i_y) \). \( c_{i\sigma}^\dagger(c_{i\sigma}) \) represents the creation (annihilation) operator on site \( i \), with \( \sigma = \uparrow, \downarrow \) being the spin of the election. The operator \( n_{i\sigma} = c_{i\uparrow}^\dagger c_{i\sigma} \) measures the number of electrons with spin \( \sigma \) on site \( i \). We set \( t \) as the energy unit in this work. The first (second) term in the Hubbard model represents the kinetic (interaction) energy. The last term is a spin-dependent potential from an external field, which is applied to explicitly break the SU(2) symmetry. We use the external field as a pinning field, applied to the edges, in such a way that the symmetry breaking allows us to measure local densities as opposed to the more demanding correlation functions [31]. As we illustrate below (Fig. 3), the effects of the pinning field are negligible in the bulk of the system. So the details of the field does not affect the characterization of the ground state. We have also tested the cases with charge pinning field alone and simultaneous spin and charge pinning field, and the results are consistent with those obtained with spin pinning field only.

To characterize the spin order, we measure the staggered spin density \( S_{\uparrow} = \frac{1}{2} \langle \sum_{i=1}^{N} c_{i\uparrow}^\dagger c_{i\uparrow} \rangle \) in the presence of the symmetry-breaking pinning field mentioned above. To characterize the charge order, we measure the local hole density \( h_i = \langle 1 - n_{i\uparrow} - n_{i\downarrow} \rangle \). We denote the average hole density, or doping, in the system as \( \delta = 1 - \frac{N_e}{N_{\text{site}}} \) where \( N_e \) is the total number of electrons and \( N_{\text{site}} = L_x \times L_y \) the number of sites of the lattice. In most calculations, a cylindrical geometry is adopted to accommodate the pinning fields. We study rectangular lattices with either open or periodic boundary conditions on the longer direction (\( x \)), and either periodic or twist boundary condition on the shorter one (\( y \)). Below when we present the results, unless otherwise specified, the default will be cylindrical cells, namely open along \( x \) and periodic along \( y \). This allows us to study systems with a size which can accommodate one or multiple periods of density waves or stripe order. We vary the aspect ratio of the simulation cells to confirm the robustness of the results, as discussed in Sec. [13]

B. AFQMC method and self-consistent constraint

We employ the constrained-path auxiliary field quantum Monte Carlo (CP AFQMC) method [11, 28] to calculate the ground state of the doped 2D Hubbard model in this work. In CP AFQMC, a trial wave-function is used to control the fermion sign problem [32, 33]. In this
work we employ trial wave functions of an unrestricted Hartree-Fock form. Recently, we developed a strategy to optimize the trial wave-function self-consistently to reduce the constraint error and to minimize the dependence of results on the trial wave-function [29]. CP AFQMC has proved to be highly accurate in several key benchmarks and, with its latest algorithmic advances, has played an important role in the recent advances in the Hubbard model [7, 30, 34].

III. DETERMINING SPIN AND CHARGE ORDERS

A. Benchmark and the effect of pinning fields

We first take the $20 \times 4$ cylinder with $U = 6$ and $\delta = 0.1$ as an example to illustrate the method and provide a sense of its procedure and accuracy. For a narrow cylindrical system such as this one, DMRG [35, 36] can provide highly accurate results for benchmark. A pinning field is applied at the edges of the cylinder to induce local antiferromagnetic order: $v_{ii} = -v_{i\uparrow} = (1)^{i_x \downarrow + i_y} v_p$ for $i_x = 1$ and $i_x = L_x$. The strength of the pinning field is $v_p = 0.5$ here.

The result for the staggered spin density is shown in Fig. 1. We start the self-consistent iteration with the free-electron ($U_{\text{eff}} = 0$) trial wave-function. The energy from the free-electron trial wave-function is $-66.74(1)$, which is very close to the exact (DMRG) energy of $-66.82(1)$. (Note that the energy computed from CP AFQMC with the so-called mixed estimate is not variational [37]). However, the staggered spin density from the free-electron trial wave-function displays some significant discrepancies with respect to the exact result as seen in Fig. 1. As detailed in [29], we set up a self-consistent loop using the CP AFQMC solution to determine a mean-field solution with an effective $U$, $U_{\text{eff}}$, which minimizes the difference between its density (or density matrix) and that from AFQMC. This solution (which has broken spin symmetry) is used as the new trial wave function, and the process is iterated to convergence. After 6 iterations, the CP AFQMC results are indistinguishable from the exact results, consistent with previous studies [29]. The result for hole density is shown in Fig. 2. There is still noticeable discrepancy in the converged local hole densities, but the pattern is the same as the exact DMRG results.

In Fig. 3 we study the effect of the strength of the pinning field on the results. The system is a $32 \times 6$ cylinder with $U = 6$ and $\delta = 1/8$. Pinning fields are applied on the two edges, similar to the setup in the previous example. The strength of the pinning field, $v_p$, is now varied by a factor of 4, from 0.2 to 0.8. We see that both the staggered spin density and hole density remain essentially unchanged in the “bulk” of the system. This validation shows the viability of probing long-range order with local pinning fields (provided that sufficiently large system sizes can be studied).
B. Finite size scaling

At each set of system parameters \((U, \delta)\), we probe the order in a range of (large) lattice sizes. A true ground-state long-range order will persist with increasing system size, while a short-range correlation induced by the local pinning field will die out as the system size grows. This is shown in Fig. 5 in which the spin orders are computed in width-8 cylinders at \(\delta = 1/12\) doping, with \(U = 2\) and \(U = 4\), respectively. At \(U = 2\) the spin density in the “bulk” of the system tends to zero as the length of the system is increased, while it is almost unchanged at \(U = 4\) for \(L_x = 24\) to 72, displaying a spin-density wave (SDW) with a consistent wavelength.

As a more quantitative probe of the order, we calculate the spin structure factor \(S_s(k) = \frac{1}{V} \sum_{\mathbf{r}_i} e^{i \mathbf{k} \cdot \mathbf{r}_i} \langle n_{i\uparrow} - n_{i\downarrow} \rangle\), where \(\mathbf{k} = (k_x, k_y)\), with \(k_x = n_x 2\pi/L_x\) and \(k_y = n_y 2\pi/L_y\) \((n_x \in [0, L_x)\) and \(n_y \in [0, L_y)\) are integers). The results are shown in Fig. 5 At \(U = 4\), a peak is seen in the spin structure factor at \(\mathbf{k}_p = ((1 - \delta)/2, \pi), \text{i.e.}, ((12\pi/7, \pi)\) in this case, which agrees with the wave-length of the SDW in Fig. 4. The height of the peak saturates among the larger supercells. At \(U = 2\), a smaller peak is also present at \(\mathbf{k}_p\). However, the value of the peak decays as system size \(L_x\) is increased.

We next perform a finite size scaling of the values of the spin structure factor at \(\mathbf{k}_p\) (the peak position). In order to reach the TDL, we extrapolate \(S_s(\mathbf{k}_p)\), first as a function of the width \(L_y\) of the system, followed by an extrapolation as a function of the length \(L_x\). This procedure is shown in Fig. 6. At \(U = 2\) (left panel), the extrapolated values for \(L_x = 24, 48\), and 72 are \(0.060(1), 0.029(5)\), and \(0.018(3)\) respectively, while at \(U = 4\) (middle panel), the corresponding values are \(0.120(5), 0.117(6)\), and \(0.125(3)\). Extrapolations of these results with \(L_x\) yield the following values of the spin structure factor at the TDL: \(-0.003(5)\) at \(U = 2\) and \(-0.123(9)\) at \(U = 4\). From these results we conclude that, for doping \(\delta = 1/12\), a spin order is absent at \(U = 2\) but present at \(U = 4\). (These two points are indicated as points A and B in the phase diagram in Fig. 5.) We systematically apply this procedure to determine the presence of order for each set of Hamiltonian parameter hence an estimate of the critical interaction strength \(U_c\) for the appearance of an SDW or stripe order, and map out a phase diagram for \(U \lesssim 12\).

C. Determining the wavelength of the collective modes

We find that a modulated spin order appears for doping values up to about \(\delta \sim 1/5\), often accompanied by charge orders. We will further discuss the properties of these collective modes and provide a detailed phase diagram below.

Here we describe our investigation of the wavelength of the collective mode in the spin and charge order in the

FIG. 3: Insensitivity of the long-range order to the strength of the local pinning field. Staggered spin density (up) and hole density (down) are shown for a \(32 \times 6\) cylinder with 1/8 doping and \(U = 6\). The strengths of the pinning field ranges from 0.2 to 0.8. Converged results from self-consistent CP AFQMC are shown for each system. The pinning field has little effect on the spin and hole density, especially in the “bulk” of the system.

FIG. 4: Presence and absence of long-range order with supercell system size. The staggered spin density is shown for two interaction strengths, \(U = 2\) (top) and \(U = 4\) (bottom), at \(\delta = 1/12\) doping, each for a sequence of supercell sizes. All results are for cylinders with width 8, and the staggered spin densities are plotted along the long \((x)\) direction. As the length of the cylinder is increased, the staggered spin density vanishes for \(U = 2\) but remains a constant for \(U = 4\).
ground state. We first illustrate the procedure using the different vertical scales in the two panels.

![Graph showing spin structure factor](image)

**FIG. 5:** Spin structure factor $S(k_x, \pi)$ for a variety of simulation cell sizes, at two interaction strengths, $U = 2$ (top) and $U = 4$ (bottom). All systems are at $\delta = 1/12$ doping. A peak is seen at $k_x = \frac{\pi}{12}$. With the increase of $L_x$, the peak decreases and vanishes at $U = 2$ but saturates at $U = 4$. Note the different vertical scales in the two panels.

Recent studies from DMRG [39] and the minimally entangled typical thermal states (METTS) [27] methods have found half-filled stripes in width-4 cylinders. For example, at $U = 12$ half-filled stripes are identified as the ground state for all doping values below $\sim 1/9$ [39], while from METTS $\delta = 1/16$ at $U = 10$ is seen to exhibit half-filled stripe order at very low temperatures [27]. Our calculations suggest that, in the pure Hubbard model, the half-filled stripe state appears to be special to width-4 cylinders, and we see filled stripes become the ground state in wider cylinders. In Fig. 8, we show an example of $\delta = 1/12$ and $U = 12$, in four different simulation cells — two width-4 cylinders, $24 \times 4$ and $48 \times 4$, and two width-8 cylinders $24 \times 8$ and $48 \times 8$. Each calculation is performed following the same procedure that we have outlined. We see that the half-filled stripe is indeed the ground state for width-4 cylinders upon convergence of the self-consistent AFQMC. For width-8 cylinders, however, the ground state corresponds to filled stripes. We also compare the computed energies of half-filled and filled stripes at $U = 12$ and $\delta = 1/12$ in Table. 4 We find that the energy for half-filled stripe is lower than that of the filled stripe in width-4 systems but this trend is reversed in width-8 systems. These results indicate that the half-filled stripes in width-4 cylinder are affected by finite size effects, and the stripes become filled at the TDL.

Recent studies in larger cells, for example using variational Monte Carlo [16], have suggested that the spin order might show wavelengths of $\alpha/\delta$, where $\alpha$ is neither 1 (half-filled) nor 2 (filled), for instance displaying a metallic state with $\alpha$ being a fraction. We searched in a few such cases but did not find a stripe state with fractional $\alpha$. Below we show an example at $U = 8$ and $\delta = 1/12$. We computed the energies using trial wave functions with several different wavelengths, without invoking the self-consistency loop in the constraint. (In these cases the QMC results turned out to stay with the same wavelength, indicating that such a state is close in energy to the true ground state, as seen from the results below.) PBC is applied along both directions and the pinning field is removed, in order to allow direct comparison of the energies. As seen in Table [11] in the $48 \times 6$ lattice, the energy from the $2/3$ filled stripe state ($\lambda = 8$) is slightly lower than filled stripe state ($\lambda = 12$), and both state are lower than half-filled stripe state ($\lambda = 6$), which is consistent with the result obtained in Ref. 10. (Note that the best variational wave function gives an energy that is $\sim 0.013t$ per site higher.) In the $48 \times 8$ lattice, the energies of the filled and $2/3$ filled stripe state are almost degenerate. We next performed a calculation with a trial wave function constructed from a linear combination of all three states, and the result is a filled stripe state. We thus conclude that, to within our resolution, the ground state is a filled stripe state.

**IV. PHASE DIAGRAM**

Using the procedure described in the previous section, we map out the phase diagram of the spin and charge orders in the ground state of the pure two-dimensional Hubbard model ($t' = 0$) in the TDL, from weak ($U \sim 0$) to fairly strong ($U \sim 12$). The results are summarized in Fig. 9. We find that, up to a doping value of $\delta \sim 0.2$, there exists a critical interaction strength $U_c(\delta)$, above
We have referred to such states as SDWs (which can have charge order). As the interaction strength is increased and the doping is reduced, the SDW states evolve into stripe states, where the holes become more and more localized at the nodes. The distinction between the SDW and stripe states is not absolute, but it is important to emphasize that a modulated AFM order can exist with two different kinds of behaviors for the holes: mobile and wavelike vs. localized and particle-like [12].

In Fig. 9 green squares represent parameters which lead to a ground state with SDW or stripe order in the TDL, while red circles represent those which do not. Within Hartree-Fock diagonal stripes are found to be more stable than linear (along x- or y-direction) stripes at large $U$ [40]; diagonal stripes were also found to be close in energy with linear stripe state in the doped t-J model [13, 41]. We searched for diagonal stripes in the Hubbard model in the parameter regime studied here, but did not find them to be the ground state. (More details are given in the appendix.) Note that results from an inhomogeneous dynamical mean-field theory (iDMFT) study [12] are in reasonable agreement with our results.

Based on our results, we show an estimate for the phase boundary as a solid black line in Fig. 9 whose position is not to be taken literally but which is bracketed by the data points around it. (In the appendix, we show two

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**TABLE I:** Comparison of the computed energies per site in the half-filled and filled stripe states at $U = 12$ and $\delta = 1/12$, in cylinders with widths 4 and 8, and lengths 24 and 48. The system setup is the same as in Fig. 8. Half-filled stripe state has lower energy in width-4 systems but higher energy in width-8 systems. A correction has been applied to the energies to account for finite Trotter step size [28].

| lattice | half-filled stripe | filled stripe |
|---------|--------------------|---------------|
| 24 × 4  | -0.5639(1)         | -0.5630(1)    |
| 48 × 4  | -0.5583(2)         | -0.5569(2)    |
| 24 × 8  | -0.5596(2)         | -0.5613(2)    |
| 48 × 8  | -0.5532(2)         | -0.5541(2)    |

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FIG. 8: Different behaviors in width-4 (top panel) and width-8 (bottom) cylinders. Staggered spin densities are shown for \( \delta = 1/12 \) doping with \( U = 12 \). The red curves show results for cylinders of length \( L_x = 24 \), while the blue curves show those with \( L_x = 48 \).

example scans, one fixed at \( U = 6 \) varying \( \delta \), and the other at \( \delta = 1/12 \) varying \( U \), to illustrate how the waves evolve across the transition line.)

From the results, we see that the critical interaction strength \( U_c(\delta) \) increase with the doping level \( \delta \). Nothing special is seen around the doping value of \( \delta = 1/8 \). The SDW or stripe order persists from small doping near half-filling to doping levels as large as \( 1/5 \).

As discussed in more detail in Sec. III C, we did not find phase separation or non-filled SDW/stripe orders which survived in our finite-size scaling procedure. This of course does not completely rule out such phases, because of the delicate nature of the different competing states and sensitivity to finite-size and other effects, as well as possible systematic errors in the calculation. However, it does provide a rather stringent screening of other possible states, given the high accuracy and extensive nature of these calculations.

V. CONCLUSION AND PERSPECTIVE

Employing state-of-the-art AFQMC methods with self-consistent constraint and performing finite-size scaling to large simulation cell sizes, we map out the ground state phase diagram of the doped 2D Hubbard model regarding the spin and charge orders as a function of doping \( \delta \) and interaction strength \( U \). Modulated SDW or stripe orders are found to exist for doping as large as \( \sim 1/5 \) with sufficiently large \( U \). The period of the spin (charge) density wave was found to be \( 2/\delta (1/\delta) \), which implies that the ground state stripes (at larger \( U \)) are filled. Our results show that stripe/SDW exists not only in the vicinity of \( 1/8 \) doping, but also extends to very small doping near half-filling and to the overdoped region. Recent experiments in cuprate [43] found that stripe order exists with doping beyond the superconducting dome, remaining observable for as large as \( \delta \approx 0.21 \). In the future, it will be interesting to study how the phase diagram changes with the inclusion of a small next-nearest hoping \( t' \). The inclusion of \( t' \) frustrates the antiferromagnetic order at

| lattice | \( \lambda = 6 \) | \( \lambda = 8 \) | \( \lambda = 12 \) |
|---------|----------------|----------------|----------------|
| 48 x 6  | -0.6820(2)    | -0.6862(2)    | -0.6855(2)    |
| 48 x 8  | -0.6821(2)    | -0.6854(2)    | -0.6852(2)    |
half-filling and we anticipate that it will cause the critical interaction $U_c$ to increase for a given doping level, and potentially change the properties of the orders. Superconductivity is found to be absent in the pure Hubbard model [31] and very recent results indicate that a small positive $t'$ can induce superconductivity in the doped $t-J$ model [44,46]. The relationship between stripe and superconductivity is an important topic for future investigation.

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Appendix A: Filling of stripes

In Fig. 10, we show additional results for the spin and hole densities in three other systems to supplement Fig. 7: $\delta = 1/10$ and $U = 5$, $\delta = 1/8$ and $U = 6$, and $\delta = 1/6$ and $U = 8$.

Appendix B: Examples of parameter scans in the phase diagram

In Fig. 11, we show how the spin and charge orders evolve as a function of $U$ at fixed doping $\delta = 1/12$. The system is a cylinder with size $8 \times 48$. A modulated AFM order develops only when $U \geq 4$. Similarly, in Fig. 12, we show the results of a scan at fixed interaction strength $U = 6$, in systems of size $L_x \times 6$, with $L_x$ from 32 to 48 to accommodate $1/16$, $1/24$, and $1/32$ dopings. As can be seen, no order is present until $\delta \leq 1/8$.

| Doping | Lattice | Linear Stripe | Diagonal Stripe |
|--------|---------|---------------|-----------------|
| $1/16$ | $32 \times 8$ | $-0.5095(2)$ | $-0.5076(1)$ |
| $1/24$ | $48 \times 6$ | $-0.4611(1)$ | $-0.4595(1)$ |
| $1/32$ | $64 \times 6$ | $-0.4371(2)$ | $-0.4362(1)$ |

TABLE III: Energy (per site) comparison for linear and diagonal stripe states at $U = 12$. The linear stripe state consistently has lower energy.

Appendix C: Diagonal vs. linear stripes

In Hartree-Fock calculations, stripe states in the diagonal direction were observed at small doping and large $U$ [40]. Studies using dynamical mean-field theory (DMFT) with exact diagonalization solvers also predicted diagonal stripes for $\delta < 0.05$ [23]. In Table. III, we present energy comparison for linear and diagonal stripe state at $U = 12$ for $1/16$, $1/24$, and $1/32$ dopings. The energies are calculated with TABC to minimize finite size effects [38]. As we can see in Table. III in our calculations the linear stripe order always has a lower energy than the diagonal stripe for doping as low as $\delta = 1/32$. Our systematic calculations at $\delta = 1/32$, $U = 2$ and $\delta = 1/24$, $U = 5$ also yielded a linear SDW or stripe state.
FIG. 10: Similar as Fig. 7. The staggered spin and charge densities are shown for 1/10 doping (U = 5), 1/8 doping (U = 6) and 1/6 doping (U = 8).

FIG. 11: Staggered spin (up) and hole (down) density at 1/12 doping for different U values. The stripe order develops with U ≥ 4.
FIG. 12: Staggered spin (up) and hole (down) density at $U = 6$ for different dopings. Order only develops with $\delta \leq 1/8$. 