Quantum Monte Carlo study of the two-dimensional fermion Hubbard Model

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We report large scale determinant Quantum Monte Carlo calculations of the effective bandwidth, momentum distribution, and magnetic correlations of the square lattice fermion Hubbard Hamiltonian at half-filling. The sharp Fermi surface of the non-interacting limit is significantly broadened by the electronic correlations, but retains signatures of the approach to the edges of the first Brillouin zone as the density increases. Finite-size scaling of simulations on large lattices allows us to extract the interaction dependence of the antiferromagnetic order parameter, exhibiting its evolution from weak-coupling to the strong-coupling Heisenberg limit. Our lattices provide improved resolution of the Green’s function in momentum space, allowing a more quantitative comparison with time-of-flight optical lattice experiments.

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I. INTRODUCTION

Originally introduced to explain magnetism and metal-insulator transitions in solids with strong electronic correlations and narrow energy bands,1–5 the underlying physics of the fermion Hubbard Hamiltonian6–9 remains a topic of considerable discussion. In two dimensions, when the lattice is doped away from half-filling, do the fermions condense into a superconducting state? If so, what is the symmetry of the pairing order parameter?10–14 Do charge inhomogeneities (stripes and checkerboards) emerge, and what is their interplay with magnetic and superconducting orders?15–18

In contrast to this uncertainty concerning the properties of the doped lattice, the qualitative behavior at half-filling (one fermion per site) is much more well understood. The interaction strength U causes both the development of long range antiferromagnetic order (LRAFO) and insulating behavior. Even so, there are still some remaining open fundamental questions, for example, in the precise way in which the model evolves from the weak-coupling to strong-coupling limits, especially in two dimensions.

At weak-coupling, one pictures the insulating behavior to arise from a Fermi-surface instability which drives LRAFO and a gap in the quasiparticle density of states. On the other hand, at strong coupling the insulating behavior is caused by Mott physics and the suppression of electron mobility to avoid double occupancy. These points of view are clearly linked, however, since for large $U/t$ the Hubbard Hamiltonian has well defined local moments and maps onto the antiferromagnetic Heisenberg model with exchange constant $J = 4t^2/U$.19

Developing an analytic theory which bridges these viewpoints quantitatively is problematic. Hartree Fock (HF) theory provides one simple point of view, but predicts LRAFO at finite temperatures in two dimensions, in violation of the Mermin-Wagner theorem. In fact, even in higher dimension when the Néel temperature $T_N$ can be nonzero, HF theory predicts $T_N \propto U$ instead of the correct $T_N \propto J = 4t^2/U$. Sophisticated approaches such as the self-consistent renormalized theory,20,21 the fluctuation-exchange approximation,22 and two-particle self-consistent theory23 obey the Mermin-Wagner theorem and provide a good description of the Hubbard Hamiltonian at weak-coupling, but fail for large $U/t$. A recent approach,24 based on the mapping to the nonlinear sigma model,25 has made some progress in connecting the two regimes.

The need to pin down the behavior of the two-dimensional (2D) half filled Hubbard model more quantitatively, in a way which links the weak-coupling and strong-coupling limits, is particularly germane at present with the achievement of cooling and quantum degeneracy in ultracold gases of fermionic atoms.26–34 Such systems offer the prospect of acting as an “optical lattice emulator” (OLE) of the fermion Hubbard model, allowing a precise comparison of experimental and theoretical phase diagrams which is difficult in the solid state, where the (single band) Hubbard Hamiltonian provides only a rather approximate depiction of the full complexity of the atomic orbitals. Obviously, the achievement of this goal is one which requires accurate computations. A particular issue in the field of OLE concerns whether the temperature dependence of the double occupancy rate changes sign during the course of the evolution from weak to strong coupling.32

It is the intent of this paper to present considerably improved results for the effective bandwidth, momentum distribution, and magnetic correlations of the square lattice fermion Hubbard Hamiltonian. We will employ the determinant quantum Monte Carlo (DQMC) method, which provides an approximation-free solution of the model, on lattices large enough to use finite-size scaling to, for example, reliably extract the antiferromagnetic order parameter as a function of interaction strength. There is a considerable existing body of QMC studies of the two-dimensional half-filled Hubbard model, both on
we show a sequence which increases the efficiency of the and "delayed updating" of the fermion at half-filling. Another single-particle site \( j \) describes a set of itinerant electrons, represented by \( c^\dagger_{j\sigma} c_{i\sigma} \), the annihilation (creation) operators at lattice site \( j \) and spin \( \sigma \). The corresponding number operator \( n_{ij\sigma} = c^\dagger_{j\sigma} c_{i\sigma} \). The first term represents the hopping (kinetic energy) of the electrons. We will choose the parameter \( t = 1 \) to set our unit of energy. The non-interacting bandwidth \( W = 8t \). \( U \) is the on-site repulsion of spin-up and spin-down electrons occupying the same lattice site, and \( \mu \) is the chemical potential which controls the particle density. We will mostly be interested in the properties of the model on \( N = L \times L \) square lattices at half-filling (the number of particles is equal to the number of lattice sites) which occurs at \( \mu = 0 \) with our particle-hole symmetric choice of the representation of the interaction term.

We will also focus exclusively on the case of the square lattice. This particular geometry has several interesting features. The half-filled square lattice Fermi surface exhibits perfect nesting, and the density of states is (logarithmically) divergent. As a consequence, the antiferromagnetic and insulating transitions occur immediately for any nonzero value of the interaction strength \( U \), instead of requiring a finite degree of correlation, as is more generically the case.

Our DQMC algorithm is based on Ref. 41 and has been refined by including "global moves" to improve ergodicity\(^{42} \) and "delayed updating" of the fermion Green’s function,\(^{43} \) which increases the efficiency of the linear algebra. Details concerning this new code are available at Ref. 44. Some other approaches to fermion Hubbard model simulations are contained in Refs. 39 and 45–47.

### III. SINGLE-PARTICLE PROPERTIES

We begin by showing single-particle properties. The momentum distribution \( n(k) = \frac{1}{2} \sum_{\sigma} \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle \) is obtained directly in DQMC via Fourier transform of the equal-time Green’s function \( G_{ji} = \langle c^\dagger_{j\sigma} c_{i\sigma} \rangle \)

\[
n(k) = 1 - \frac{1}{2N} \sum_{i,j,\sigma} \langle c^\dagger_{k\sigma} c_{i\sigma} \rangle \cdot \left( \langle c^\dagger_{j\sigma} c_{i\sigma} \rangle \right). \tag{2}
\]

At \( U = 0 \) and at half-filling, \( n(k) = 1(0) \) inside (outside) a square with vertices \((\pi, 0), (0, \pi), (\pi, 0), (0, -\pi)\) within the Brillouin zone (BZ). In Fig. 1(a), we show \( n(k) \) around the complete BZ, while Fig. 1(b) focuses on the region near the Fermi-surface point \((\pi, 2, \pi/2)\). Interactions broaden the \( U = 0 \) Fermi surface considerably. Figure 1(c) shows that data for different lattice sizes fall on the same curve. Smearing due to finite temperature effects is seen in Fig. 1(d) to be small below \( T = t/\beta = 8 \).

Recent optical lattice experiments\(^{29} \) have imaged this Fermi surface for a three-dimensional cloud of fermionic \(^{40} \)K atoms prepared in a balanced mixture of two hyperfine states which act as the Hubbard Hamiltonian spin degree of freedom. In Fig. 2 we show a sequence of color contour plots for different densities at weak and intermediate couplings, \( U/t = 2, 4 \). As in the experiments, and in agreement with Fig. 1, the Fermi surface may still be clearly discerned, and evolves from a circular topology at low densities into the rotated square as the BZ boundaries are approached. Because of the sign problem\(^{48, 49} \) which occurs in the doped system, the temperatures shown in the figure are rather higher than those used in Fig. 1 at half-filling. Another single-particle
quantity of interest is the effective hopping,

$$\frac{t_{\text{eff}}}{t} = \frac{\langle c_{j+\hat{x}\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{j+\hat{x}\sigma} \rangle_U}{\langle c_{j+\hat{x}\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{j+\hat{x}\sigma} \rangle_{U=0}}$$

which measures the ratio of the kinetic energy at finite $U$ to its non-interacting value. As the electron correlations grow larger, hopping is increasingly inhibited, and $t_{\text{eff}}$ is diminished. In Fig. 3, we show a plot of this ratio as a function of $U$ for a $10 \times 10$ lattice. Note that despite the insulating nature of the system, the effective hopping is nonzero and does not serve as an order parameter for the metal-insulator transition. Indeed, $t_{\text{eff}}$ is responsible for the superexchange interaction which drives antiferromagnetic order. The effective hopping can be evaluated analytically at small and large $U$. The DQMC data interpolates between these two limits.

IV. MAGNETIC CORRELATIONS

We turn now to two-particle properties, focusing on the magnetic behavior. The real-space spin-spin correlation
For a \( 24 \times 24 \) lattice, all temperatures, and saturation is visible at \( \beta t \) in the inset. Anti-ferromagnetic correlations are present for horizontal axis follows the triangular path on the lattice shown in the inset. The on-site repulsion \( U \) suppresses the doubly occupied configuration and hence also the empty one, if the total occupation is fixed at one fermion per site. Ultimately, charge fluctuations are completely eliminated, \( \langle m^2 \rangle \rightarrow 1 \) and the Hubbard model maps onto the spin-\( \frac{1}{2} \) Heisenberg Hamiltonian. This is illustrated in Fig. 4 for a \( 10 \times 10 \) lattice. By the time \( U = W = 8t \), the local moment has attained 90% of its full value. Thermal fluctuations also inhibit local moment formation but the data shown for function. The singly occupied states \( |\uparrow\rangle \) and \( |\downarrow\rangle \) have \( \langle m^2 \rangle = 1 \) while the empty and doubly occupied ones \( |0\rangle \) and \( |\uparrow\downarrow\rangle \), have \( \langle m^2 \rangle = 0 \). In the non-interacting limit, at half-filling, each of the four possible site configurations is equally likely. Hence the average moment \( \langle m^2 \rangle = \frac{1}{4} \). The local moment has \( \langle m^2 \rangle = 0 \) at low temperatures. Anti-ferromagnetic correlations are present for all temperatures, and saturation is visible at \( \beta t = 32 \).
different temperatures in Fig. 4 indicate they are mostly eliminated by the time \( T \) decreases below \( t/12 = W/96 \).

Local moments provide an intuitive picture of the onset of long-range correlation in the strong-coupling regime. They first form on the temperature scale \( U \), which acts to eliminate double occupancy, and then, at yet lower \( T \), they order via antiferromagnetic exchange interaction with \( J = 4t^2/U \). In contrast with this situation, weak-coupling correlations are better described as arising from the instability of the Fermi gas against formation of a spin-density wave, a peculiarity of the square lattice, suggesting an ordering temperature proportional to \( U \).

Figure 5 shows the spin-spin correlation function in the latter regime (\( U = 2 \)) for a \( 20 \times 20 \) lattice at \( \beta t = 12 \) and 32. The correlations extend over the entire lattice even at \( \beta t = 12 \), i.e., the correlation length has become comparable to the system size already at this temperature. The values of \( C(1) \) continue to grow as \( T \) is increased further, saturating at \( \beta t \approx 32 \). This observation disproves the commonly held idea that on finite clusters, the order parameter stop growing after the correlation length exceeds the linear size of the system. Such saturation happens at a much lower temperature, only after thermal fluctuations have been largely eliminated.

A comparison of \( |C(1)| \) for \( U = 2 \) and different lattice sizes is given in Fig. 6, where data for \( L = 8 \) up to \( L = 24 \) are plotted and we have taken the absolute value to make the convergence with \( L \) clearer. We have fixed \( \beta t = 32 \) so the spin correlations have reached their asymptotic low-temperature values. As expected, the smallest lattice sizes (\( 8 \times 8 \)) overestimate the tendency to order, with \( |C(1)| \) significantly larger than for values of larger \( L \). However, by the time \( L = 20 \) the finite-size effects are small.

We next compare the spin-spin correlation function for various \( U \) at low temperatures on a \( 24 \times 24 \) lattice in Fig. 7. Long-range order is present at all interaction strengths. For each \( U \), we have chosen temperatures such that the ground state has been reached for this lattice size. Since statistical fluctuations increase significantly with \( U \) and with \( \beta \) in DQMC, it is advantageous not to simulate unnecessarily cold systems. As discussed above, such temperature should increase with \( U \) in the weak-coupling regime and scale proportionally to \( 1/U \) in the strong-coupling one. We indeed find the highest saturation temperatures in the intermediate regime, at \( U/t \approx 4 \).

The magnetic structure factor \( S(k) \) is the Fourier transform of the real-space spin-spin correlation function \( C(1) \),

\[
S(k) = \sum_{l} e^{i k \cdot l} C(l),
\]

were \( S(k) \) is plotted in Fig. 8 as a function of \( k \) for several lattice sizes with \( U = 2t \) and \( \beta t = 32 \). \( S(k) \) is small and lattice size independent away from the ordering vector \( k = Q \equiv (\pi, \pi) \). The sharp peak at \( Q \) emphasizes the antiferromagnetic nature of the correlations on a half-filled lattice.

In order to understand the implications of the lattice size dependence at the ordering vector in Fig. 8, we show in Fig. 9 the antiferromagnetic structure factor for \( U = 2t \) as a function of inverse temperature for various \( L \). As expected, as \( L \) increases, a larger value of \( \beta \) is required to eliminate the low-lying spin-wave excitations and to saturate the structure factor to its ground state value.

It is seen from Eq. (5) that \( S(Q) \) will grow linearly with the number of sites \( N = L^2 \) if there is long-range antiferromagnetic order. Huse\(^{50} \) has used spin-wave theory to work out the first correction to this scaling,

\[
\frac{S(Q)}{L^2} = \frac{m^2}{3} + \frac{a}{L},
\]
Here $m_{af}$ is the antiferromagnetic order parameter. $m_{af}$ can also be extracted from the spin-spin correlation function between the two most distant points on a lattice, $C(L/2, L/2)$, with a similar spin-wave theory correction,

$$C(L/2, L/2) = \frac{m_{af}^2}{3} + \frac{b}{L}. \quad (7)$$

We expect that the correction $b < a$ since the structure factor includes spin correlations at short distances which markedly exceed $m_{af}^2$, in addition to the finite lattice effects at larger length scales. For similar reasons $S$ is expected to show larger corrections to the asymptotic $1/L$ scaling behavior than $C$. Part of the origin of these corrections is trivial and evident from Fig. 6: $S$

is the average of quantities as different as $C(0,0)$ and $C(L/2, L/2)$. In the large $L$ limit, $S$ and its $1/L$ finite-size error are dominated by the contribution of the large distance correlations but for small $L$ a bias roughly proportional to

$$\frac{C(0,0) - C(L/2, L/2)}{L^2} \quad (8)$$

is clearly present. This bias is larger for small $U$ since the numerator in Eq. (8) gets smaller with increasing $U$ and saturates to the value of the Heisenberg model at $U/t \approx 8$. On the other hand, the error bars on $S$ are often significantly smaller than on $C$, a fact that is certainly advantageous in the final finite-size scaling analysis.

A measure of magnetic order that incorporates the extended linearity of $C$ and the better statistical property of $S$ is given by

$$S_n(Q) = \frac{L^2}{L^2 - n} \sum_{l > l_c} c^{lQ} C(1), \quad (9)$$

where $n$ is the number of distances shorter than $l_c$. Equation (9) is nothing but the interpolation between $S$, corresponding to $n = 0$, and $C$, the case of $n = L^2 - 1$. Figure 10(a) shows how the $L \to \infty$ extrapolation evolves by increasing $l_c$. When $l_c$ is small the linear extrapolation is significantly biased by the small-$L$ results. As $l_c$ increases one reaches statistical convergence already for $l_c = 1$ (corresponding to $n = 5$, the cluster formed by the origin and the nearest neighbors) with minimal loss of statistical precision. That $l_c = 1$ is all is needed

FIG. 10: (Color online) Scaling results for $U = 5t$ and $\beta t = 20$. (a) Convergence of the extrapolated value of $S_n(Q)$ as a function of the size of the excluded cluster. See Eq. (9) for the definition of $S_n$. A large fraction of the $1/L^2$ bias is removed without loss in precision. $C(L/2, L/2)$ is plagued by a much larger error bar. (b) Scaling of $S_n(Q)$ for $n = 0, 1, 5$ and $C(L/2, L/2)$ as a function of the inverse linear lattice size. The extrapolation was performed via a linear least-squares fit in all cases.

FIG. 11: (Color online) Order parameter $m_{af}$ as a function of the interaction strength $U$. Earlier DQMC values (Ref. 51) are circles and Hartree-Fock theory scaled by the Heisenberg result from Ref. 48 are shown as a line with long dashes. The line with short dashes and the dashed and dotted line indicate the strong-coupling Heisenberg limits from QMC (Ref. 52 and spin-only low-energy theory with ring exchange (Ref. 53), respectively. Also shown is the RPA calculation of Ref. 54 (solid line).
to reach statistical convergence is also manifest in Fig. 6 where $C(1)$ drops to almost a constant beyond this value.

In Fig. 10(b) we show $S_n(Q)/L^2$ versus inverse linear lattice size $1/L$ for $U = 5t$ and $n = 0$, 1, and 5 since as shown in Fig. 10(a), there is no real gain in accuracy by excluding larger subclusters. The inverse temperatures is $\beta t = 20$, so that $S$ has reached its zero-temperature value regardless of $L$. We have repeated this finite-size scaling analysis for couplings $U/t = 2, 3, 4, 6.7$, and 8 and extrapolated to infinite $L$ using a linear least-square fit in $1/L$. In Fig. 11, we show the resulting antiferromagnetic order parameter $n_{\text{MF}}$ as a function of $U/t$ employing the same normalization convention of the other Hubbard model studies reported in this figure. The early DQMC values obtained by Hirsch and Tang, which are consistent with the ones obtained here, are shown.

Figure 11 also summarizes a number of the available analytic treatments. The line with long dashes is the random-phase-approximation (RPA) treatment in which the single-particle propagators in the usual RPA sum are also dressed by the one-loop paramagnon correction to their self-energy. Also shown (line with dots and dashes) are the results of a spin-only low energy theory which includes not only the usual Heisenberg value determined by Sandvik but also all higher order (e.g., ring exchange) terms up to $t^4/U^3$. Finally, the line with short dashes is the Heisenberg value determined by Sandvik.

\section{V. SUMMARY}

In this paper we have presented the results of determinant quantum Monte Carlo calculations for the magnetic properties of the half-filled square lattice Hubbard Hamiltonian. DQMC allows us to bridge the weak-coupling and strong-coupling regimes with a single methodology and a particular outcome of our work has been the calculation of the antiferromagnetic order parameter in the ground state as a function of $U/t$. We expect these values will be useful in validating OLE experiments on the fermion Hubbard model.

By using an improved DQMC code, we have been able to provide results on larger lattices than those originally explored. This not only has allowed us to do accurate finite-size scaling for the order parameter but we also obtain considerably better momentum resolution and hence a description of the Green’s function $G(k)$ which also offers the prospect of improved contact with time-of-flight images from optical lattice emulators.

This study demonstrates a significantly improved capability to simulate interacting fermion systems, driven by more powerful hardware as well as algorithmic advances. Systems of 500 sites (fermions) can now be handled on a modest cluster of desktop computers. Larger system simulations can easily be contemplated using more powerful hardware and would scale as the cube of the number of particles, in the absence of the sign problem. This remaining sign problem bottleneck prevents the study of the densities of most interest to high-temperature superconductivity, i.e., dopings of $5 \sim 15\%$ away from half-filling and motivates the interest in analog computation for the Hubbard Hamiltonian. It should be noted, however, that the sign problem can be rather modest for other densities, e.g., quarter filling, where we now have the capability to undertake large scale studies.

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37. The development of this new determinant Quantum Monte Carlo program is part of the DOE SciDAC program. Quantum Electron Simulation Toolbox (QUEST) is a FORTRAN 90/95 package using new algorithms, such as delayed updating, and integrating modern BLAS/LAPACK numerical kernels. QUEST has integrated several legacy codes by modularizing their computational components for ease of maintenance and program interfacing. QUEST also allows general lattice geometries. The current version can be accessed via [http://www.cs.ucdavis.edu/~bai/QUEST](http://www.cs.ucdavis.edu/~bai/QUEST).
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