

**Quantum Monte Carlo study of the two-dimensional fermion Hubbard model**C. N. Varney,<sup>1</sup> C.-R. Lee,<sup>2</sup> Z. J. Bai,<sup>3</sup> S. Chiesa,<sup>1</sup> M. Jarrell,<sup>4</sup> and R. T. Scalettar<sup>1</sup><sup>1</sup>*Department of Physics, University of California, Davis, California 95616, USA*<sup>2</sup>*Department of Computer Science, National Tsing Hua University, Hsinchu, Taiwan 30013, Republic of China*<sup>3</sup>*Department of Computer Science, University of California, Davis, California 95616, USA*<sup>4</sup>*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA*

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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 noninteracting 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,<sup>1–5</sup> the underlying physics of the fermion Hubbard Hamiltonian<sup>6–9</sup> 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?<sup>10–14</sup> Do charge inhomogeneities (stripes and checkerboards) emerge and what is their interplay with magnetic and superconducting orders?<sup>15–18</sup>

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  $J=4t^2/U$ .<sup>19</sup>

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,<sup>20,21</sup> the fluctuation-exchange approximation,<sup>22</sup> and two-particle self-consistent theory<sup>23</sup> 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<sup>24</sup> based on the mapping to the nonlinear sigma model<sup>25</sup> 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.<sup>26–31</sup> 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.<sup>32</sup>

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 finite lattices and in infinite dimension. A partial list includes Refs. 13, 18, and 33–40.

**II. MODEL AND COMPUTATIONAL METHODS**

The fermion Hubbard Hamiltonian,

$$\begin{aligned}
 H = & -t \sum_{\langle ij \rangle \sigma} (c_{j\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{j\sigma}) + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) \\
 & - \mu \sum_{i\sigma} n_{i\sigma},
 \end{aligned} \quad (1)$$

describes a set of itinerant electrons, represented by  $c_{j\sigma}$  ( $c_{j\sigma}^\dagger$ ), the annihilation (creation) operators at lattice site  $\mathbf{j}$  and spin  $\sigma$ . The corresponding number operator  $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$ . 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 noninteracting 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<sup>42</sup> and ‘‘delayed updating’’ of the fermion Green’s function,<sup>43</sup> 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  $n(\mathbf{k}) = \frac{1}{2} \sum_{\sigma} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle$  is obtained directly in DQMC via Fourier transform of the equal-time Green’s function  $G_{ji} = \langle c_{j\sigma} c_{i\sigma}^\dagger \rangle$

$$n(\mathbf{k}) = 1 - \frac{1}{2N} \sum_{i,j,\sigma} e^{i\mathbf{k}\cdot(\mathbf{j}-\mathbf{i})} \langle c_{j\sigma} c_{i\sigma}^\dagger \rangle. \quad (2)$$

At  $U=0$  and at half-filling,  $n(\mathbf{k})=1(0)$  inside (outside) a square with vertices  $(\pi,0)$ ,  $(0,\pi)$ ,  $(-\pi,0)$ , and  $(0,-\pi)$  within the Brillouin zone (BZ). In Fig. 1(a), we show  $n(\mathbf{k})$  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  $T=t/8$  ( $\beta t=8$ ).

Recent optical lattice experiments<sup>29</sup> have imaged this Fermi surface for a three-dimensional cloud of fermionic <sup>40</sup>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,  $U/t$

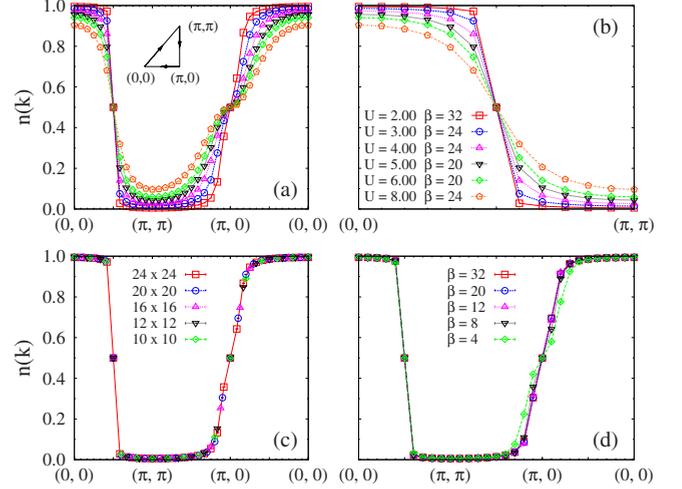


FIG. 1. (Color online) [(a) and (b)] The momentum distribution, Eq. (2), is shown for interaction strengths  $U$  ranging from  $U=2t$  (one quarter the bandwidth) to  $U=W=8t$ . A sharp Fermi surface is seen at weak-coupling as the momentum cuts across the Fermi surface at  $\mathbf{k}=(\pi/2, \pi/2)$ . Larger  $U$  broadens  $n(\mathbf{k})$  considerably. The occupation becomes substantial outside the nominal Fermi surface. Panel (a) shows the full BZ while panel (b) provides higher resolution for the portion of the cut perpendicular to the Fermi surface at  $(\pi/2, \pi/2)$ . (c) At  $U=2t$  and  $\beta t=32$ ,  $n(\mathbf{k})$  has only a weak lattice size dependence, apart from the better resolution as  $L$  increases. (d) For  $U=2t$  on a  $20 \times 20$  lattice,  $n(\mathbf{k})$  is converged to its low-temperature value once  $T < t/8$ . (By contrast, the spin correlations reach their ground-state values only at considerably lower  $T$ .)

$=2, 4$ . 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<sup>48,49</sup> 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,

$$\frac{t_{\text{eff}}}{t} = \frac{\langle c_{\mathbf{j}+\hat{x}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{j}+\hat{x}\sigma} \rangle_U}{\langle c_{\mathbf{j}+\hat{x}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{j}+\hat{x}\sigma} \rangle_{U=0}}, \quad (3)$$

which measures the ratio of the kinetic energy at finite  $U$  to its noninteracting 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  $U$ .<sup>10</sup> The DQMC data interpolates between these two limits.

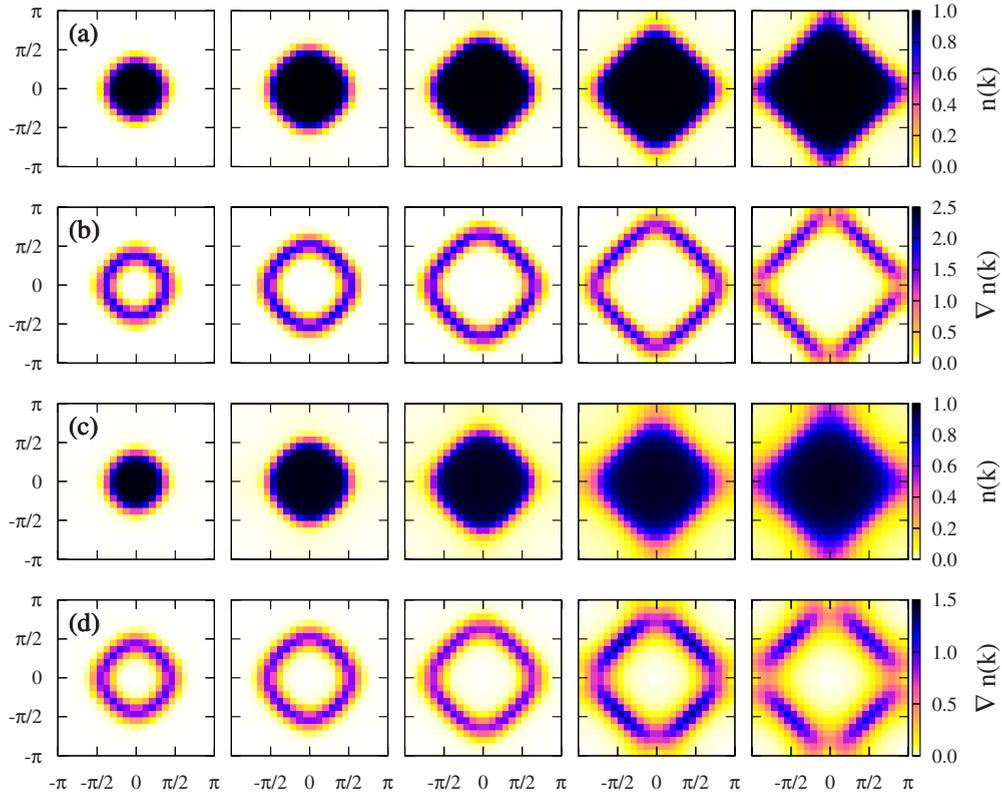


FIG. 2. (Color online) Color contour plot depiction of the momentum distribution  $n(\mathbf{k})$  and its gradient  $\nabla n(\mathbf{k})$ . (a) Left to right,  $n(\mathbf{k})$  at weak-coupling  $U=2t$  and fillings  $\rho=0.23, 0.41, 0.61, 0.79$ , and  $1.0$ . (b)  $\nabla n(\mathbf{k})$  for the same parameters. [(c) and (d)] Intermediate coupling  $U=4t$  and fillings  $\rho=0.21, 0.41, 0.59, 0.79$ , and  $1.0$ . The increased breadth of the Fermi surface with interaction strength is evident. The lattice size= $24 \times 24$  and inverse temperature  $\beta t=8$  except at  $U=4t$  and fillings  $\rho=0.59$  and  $0.79$ , where the sign problem restricts the simulation to inverse temperatures  $\beta t=6$  and  $4$ , respectively.

#### IV. MAGNETIC CORRELATIONS

We turn now to two-particle properties, focusing on the magnetic behavior. The real-space spin-spin correlation function is defined as

$$C(\mathbf{l}) = \langle (n_{\mathbf{j}+\mathbf{l}\uparrow} - n_{\mathbf{j}+\mathbf{l}\downarrow})(n_{\mathbf{j}\uparrow} - n_{\mathbf{j}\downarrow}) \rangle \quad (4)$$

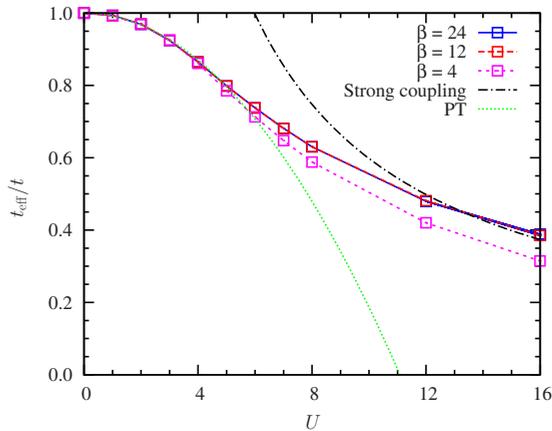


FIG. 3. (Color online) As the interaction energy  $U$  increases, the kinetic energy declines. Here we show  $t_{\text{eff}}/t$ , the ratio between the expectation value of  $\langle c_{\mathbf{j}+\mathbf{x}\sigma}^\dagger c_{\mathbf{j}\sigma} \rangle$  at  $U$  with its value at  $U=0$  for a  $10 \times 10$  lattice. Strong-coupling and perturbative graphs are also shown for  $\beta t=12$ .

and measures the extent to which the  $z$  component of spin on site  $\mathbf{j}$  aligns with that on a site a distance  $\mathbf{l}$  away. Although defined in Eq. (4) using the  $z$  direction,  $C(\mathbf{l})$  is rotationally invariant and in fact, we measure all three components to monitor ergodicity in our simulations and average over all directions to provide an improved estimator for the magnetic properties.

The local moment  $\langle m^2 \rangle = C(0,0) = \langle (n_{\mathbf{j}\uparrow} - n_{\mathbf{j}\downarrow})^2 \rangle$  is the zero separation value of the spin-spin correlation 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 noninteracting limit, at half-filling, each of the four possible site configurations is equally likely. Hence the average moment  $\langle m^2 \rangle = \frac{1}{2}$ .

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 different temperatures in

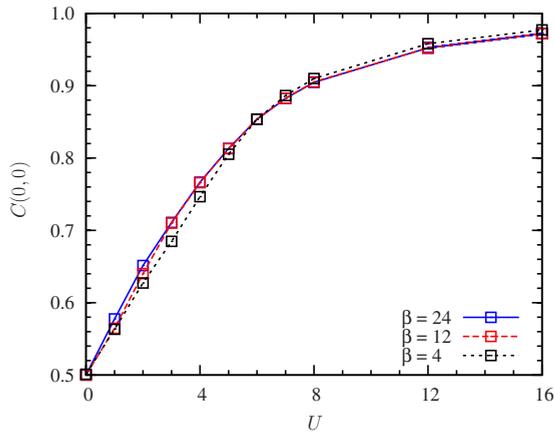


FIG. 4. (Color online) The local moment  $\langle m^2 \rangle$  is the zero spatial separation value of the spin-spin correlation function  $C(0,0)$ . In the noninteracting limit  $\langle m^2 \rangle = \frac{1}{2}$ . As the interaction energy  $U$  increases,  $\langle m^2 \rangle$  approaches 1, indicating the complete absence of double occupancy and a well-formed moment on each site.

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  $\beta t=12, 20$ , 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

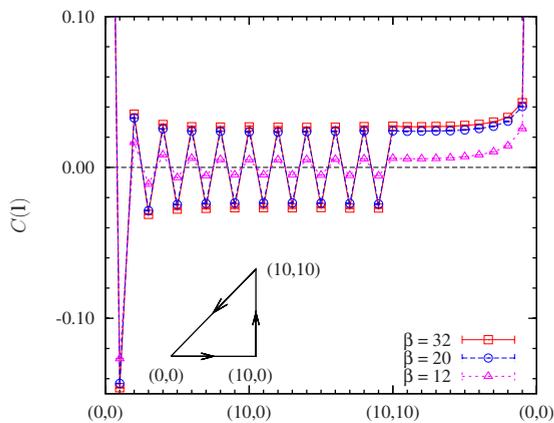


FIG. 5. (Color online) Comparison of the equal-time spin-spin correlation function  $C(\mathbf{l})$  on a  $20 \times 20$  lattice with  $\langle n \rangle = 1$  and  $U = 2t$  for inverse temperatures  $\beta t = 12, 20$ , and  $32$ . The horizontal axis follows the triangular path on the lattice shown in the inset. Antiferromagnetic correlations are present for all temperatures and saturation is visible at  $\beta t = 32$ .

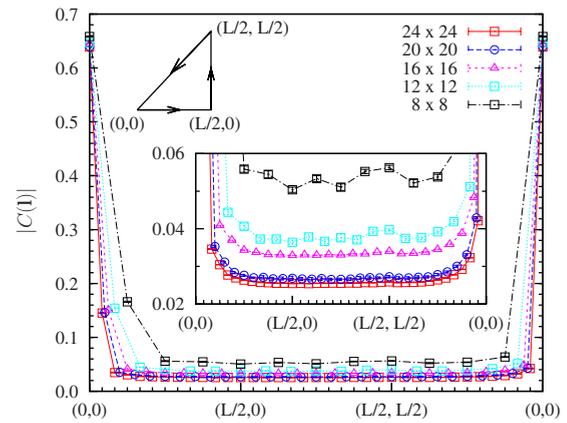


FIG. 6. (Color online) Comparison of the absolute value of the equal-time spin-spin correlation function  $C(\mathbf{l})$  at  $U=2t$  and  $\beta t=32$  for  $L \times L$  lattices with  $L=8, 12, 16, 20$ , and  $24$ . The inset is a closeup view of the long-range correlations.

$C(\mathbf{l})$  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  $|C(\mathbf{l})|$  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 with  $L$  clearer. We have fixed  $\beta t=32$  so the spin correlations with  $L$  clearer. As expected, the smallest lattice sizes ( $8 \times 8$ ) overestimate the tendency to order, with  $|C(\mathbf{l})|$  significantly larger than values for 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

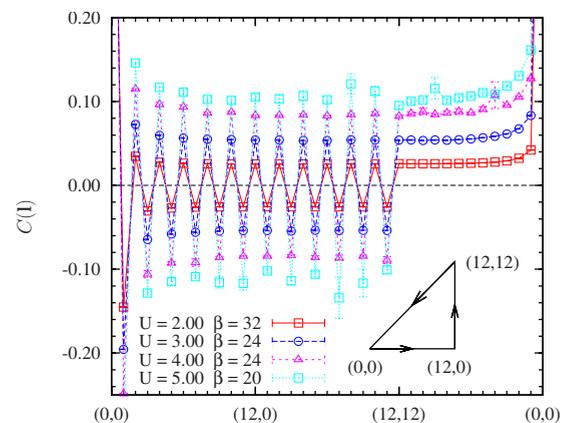


FIG. 7. (Color online) The equal-time spin-spin correlation function  $C(\mathbf{l})$  on a  $24 \times 24$  lattice with  $\langle n \rangle = 1$ . Data are shown for various  $U$  at low temperatures. Antiferromagnetic correlations are enhanced for larger values of  $U$ . The increase in statistical fluctuations with interaction strength in the DQMC method is evident.

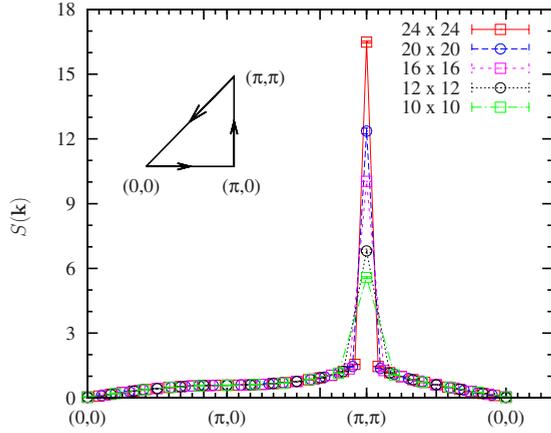


FIG. 8. (Color online) The magnetic correlation function  $S(\mathbf{k})$  for  $U=2t$  and  $\beta t=32$ . The horizontal axis traces out the triangular path shown in the inset. The function is sharply peaked at  $\mathbf{k}=\mathbf{Q} \equiv (\pi, \pi)$ .

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  $S(\mathbf{k})$  is the Fourier transform of the real-space spin-spin correlation function  $C(\mathbf{l})$ ,

$$S(\mathbf{k}) = \sum_{\mathbf{l}} e^{i\mathbf{k}\cdot\mathbf{l}} C(\mathbf{l}), \quad (5)$$

where  $S(\mathbf{k})$  is plotted in Fig. 8 as a function of  $\mathbf{k}$  for several lattice sizes with  $U=2t$  and  $\beta t=32$ .  $S(\mathbf{k})$  is small and lattice size independent away from the ordering vector  $\mathbf{k}=\mathbf{Q} \equiv (\pi, \pi)$ . The sharp peak at  $\mathbf{Q}$  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  $S(\mathbf{Q})$  will grow linearly with the number of sites  $N=L^2$  if there is long-range antiferromagnetic order. Huse<sup>50</sup> has used spin-wave theory to work out the first correction to this scaling,

$$\frac{S(\mathbf{Q})}{L^2} = \frac{m_{\text{af}}^2}{3} + \frac{a}{L}. \quad (6)$$

Here  $m_{\text{af}}$  is the antiferromagnetic order parameter.  $m_{\text{af}}$  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,

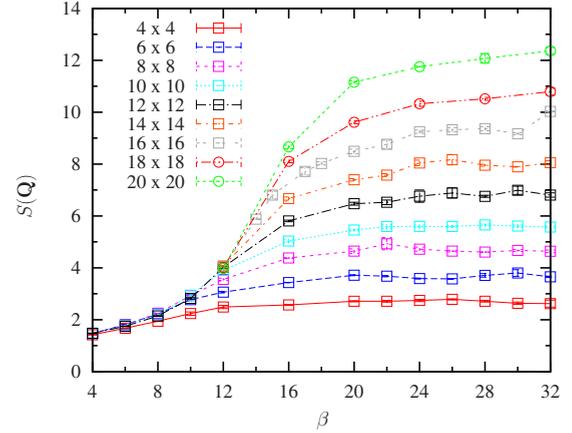


FIG. 9. (Color online) The antiferromagnetic structure factor  $S(\mathbf{Q})$  as a function of inverse temperature at  $U=2t$  for  $L \times L$  lattices with  $L=4, 6, 8, 10, 12, 14, 16, 18$ , and  $20$ .

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

We expect that the correction  $b < a$  since the structure factor includes spin correlations at short distances which markedly exceed  $m_{\text{af}}^2$ , 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

$$S_n(\mathbf{Q}) = \frac{L^2}{L^2 - n} \sum_{\mathbf{l}, l > l_c} e^{i\mathbf{Q}\cdot\mathbf{l}} C(\mathbf{l}), \quad (9)$$

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  $L \rightarrow \infty$  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 that is needed to reach statistical convergence is also manifest in Fig. 6 where  $C(\mathbf{l})$  drops to almost a constant beyond this value.

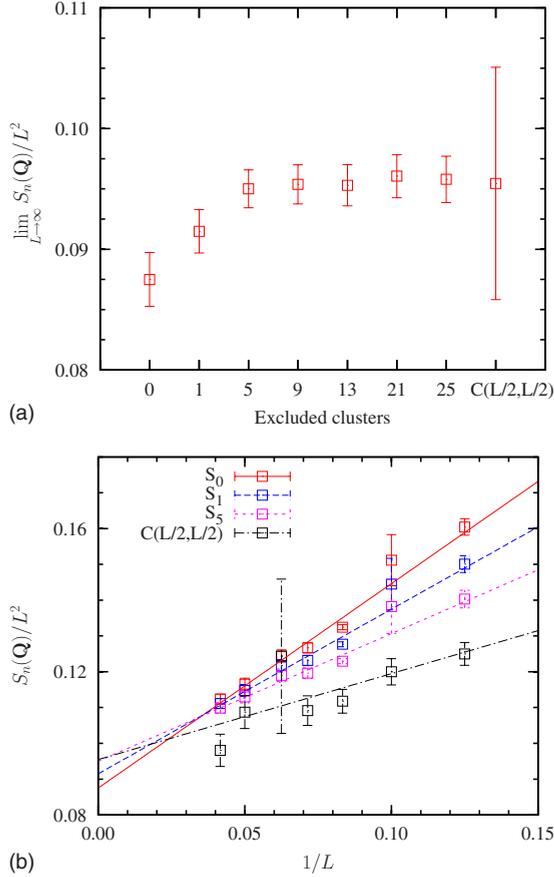


FIG. 10. (Color online) Scaling results for  $U=5t$  and  $\beta t=20$ . (a) Convergence of the extrapolated value of  $S_n(\mathbf{Q})$  as a function of the size of the excluded cluster. See Eq. (9) for the definition of  $S_n$ . A large fraction of the  $1/L^2$  bias is removed without loss in precision.  $C(L/2, L/2)$  is plagued by a much larger error bar. (b) Scaling of  $S_n(\mathbf{Q})$  for  $n=0, 1$ , and  $5$  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.

In Fig. 10(b) we show  $S_n(\mathbf{Q})/L^2$  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 temperature 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  $m_{\text{af}}$  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,<sup>51</sup> 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 result of Hartree-Fock theory scaled by the Heisenberg result at strong coupling.<sup>48</sup> The solid line 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.<sup>54</sup> Also shown (line with dots and dashes) are the results of a spin-

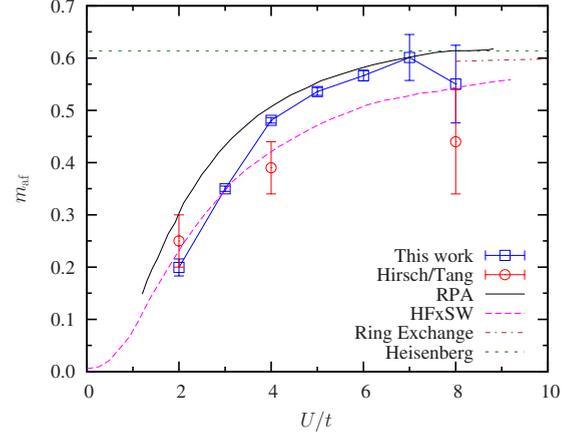


FIG. 11. (Color online) Order parameter  $m_{\text{af}}$  as a function of the interaction strength  $U$ . Earlier DQMC values (Ref. 51) are circles and Hartree-Fock theory scaled by the Heisenberg result from Ref. 48 are shown as a line with long dashes. The line with short dashes and the dashed and 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).

only low-energy theory<sup>53</sup> which includes not only the usual Heisenberg  $J=4t^2/U$  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.<sup>52</sup>

## 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 also able to provide results on larger lattices than those originally explored.<sup>10</sup> This not only has allowed us to do more 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  $G(\mathbf{k})$  which also offers the prospect of improved contact with time-of-flight images from optical lattice emulators.<sup>28–31</sup>

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 5–15 % away from half-filling and motivates the interest in

analog computation for the Hubbard Hamiltonian.<sup>55</sup> 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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<sup>44</sup>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/>  
<sup>45</sup>A useful collection of lectures summarizing some of the alternate approaches to Hubbard model QMC is contained in the NATO Advanced Study Institute: Quantum Monte Carlo Methods in Physics and Chemistry (1998), available at <http://www.phys.uri.edu/nigh/QMC-NATO/webpage/abstracts/lecturers.html>. These include "Phase Separation in the 2D Hubbard Model: A Challenging Application of Fixed-Node QMC," (Bachelet); "Quantum Monte Carlo for Lattice Fermions," (Muramatsu); and "Constrained Path Quantum Monte Carlo for Fermions," (Zhang).  
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