Competing Orders in the 2D Half-Filled SU(2N) Hubbard Model through the Pinning-Field Quantum Monte Carlo Simulations

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We nonperturbatively investigate the ground state magnetic properties of the 2D half-filled SU(2N) Hubbard model in the square lattice by using the projector determinant quantum Monte Carlo simulations combined with the method of local pinning fields. Long-range Néel orders are found for both the SU(4) and SU(6) cases at small and intermediate values of U. In both cases, the long-range Néel moments exhibit nonmonotonic behavior with respect to U, which first grow and then drop as U increases. This result is fundamentally different from the SU(2) case in which the Néel moments increase monotonically and saturate. In the SU(6) case, a transition to the columnar dimer phase is found in the strong interaction regime.

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The ultracold atom systems have opened up a wonderful opportunity for studying novel phenomena that are not easily accessible in usual solid state systems. For example, the large-spin ultracold alkali-metal and alkaline-earth-metal fermions exhibit quantum magnetic properties fundamentally different from the large-spin solid state systems such as transition metal oxides [1]. In solids, Hund's rule coupling combines several electrons on the same cation site into states carrying large spin S. However, the symmetry of these systems is usually only SU(2). The leading order coupling between two neighboring sites is mediated by exchanging one pair of electrons no matter how large S is; thus, quantum spin fluctuations are suppressed by the $1/S$ effect. In contrast, large-hyperfine-spin ultracold fermion systems which means thats of SU$(2N)$ and Sp$(2N)$. For the simplest case of spin $\frac{3}{2}$, a generic Sp(4) symmetry was proved without fine tuning, which includes the SU(4) symmetry as a special case [2]. Such a high symmetry gives rise to exotic properties in quantum magnetism and pairing superfluidity [3–12]. Furthermore, large-spin alkaline-earth-metal fermion systems have been experimentally realized in recent years [13–15]. In particular, a SU(6) Mott insulator of ^{173}Yb has also been observed [1,16]. The above theoretical and experimental progress has stimulated a great deal of interest in exploring novel properties of strongly correlated systems with high symmetries [17–23].

The SU$(2N)$ Heisenberg model was first introduced into condensed matter physics to apply the large-N technique to systematically handle strong correlation effects in the context of high T_c cuprates [24–28]. It was found that on 2D bipartite lattices the SU(2) Heisenberg model displays long-range Néel ordering [29]. As $2N$ increases, enhanced quantum fluctuations suppress Néel ordering and the ground states eventually become dimerized [27,28]. This transition has been observed by quantum Monte Carlo (QMC) simulations [30–35] for certain representations of the SU$(2N)$ symmetry [36]. However, for the self-conjugate representations, a consensus has not been achieved yet. A variational Monte Carlo study [34] found Néel ordering when $2N = 2$ and 4, and columnar dimer ordering for $2N \geq 6$. However, in a determinant QMC calculation [35], dimer ordering was found at $2N \geq 6$ in agreement with the variational QMC study, while for the SU(4) case, neither Néel nor dimer ordering exists in the Heisenberg limit.

The above Heisenberg-type models neglect charge fluctuations. The interplay between charge and spin degrees of freedom is contained in the SU$(2N)$ Hubbard model [21,37,38]. However, owing to the lack of nonperturbative methods, the SU$(2N)$ Hubbard model receives much less attention. To the best of our knowledge, a systematic nonperturbative study of the ground state properties of the 2D half-filled models is still missing. It is even not clear whether Néel or dimer ordering exists in the weak-, intermediate-, and strong-coupling regimes, respectively.

In this Letter, we perform a nonperturbative determinant QMC study on the half-filled SU$(2N)$ Hubbard model in the 2D square lattice. The ground state magnetic properties are investigated by using the local pinning-field method, which directly measures the spatial decay of the induced order parameters [39]. Long-range Néel order is identified at weak and intermediate values of U in the SU$(2N)$ Hubbard models of $2 \leq 2N \leq 6$ we studied. In the cases of SU(4) and SU(6), the Néel moments first grow then drop with increasing U. Furthermore, a transition from the Néel-ordering phase into the columnar dimer-ordering phase is observed at a large value of U in the SU(6) case. This transition is conceivably owing to the competition between

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the weak-coupling physics of Fermi surface nesting and strong coupling local moment physics.

We consider the SU$(2N)$ Hubbard model in the 2D square lattice with the periodic boundary condition as

$$H = -t \sum_{\langle i,j \rangle, \alpha} (c_{i\alpha}^{\dagger} c_{j\alpha} + \text{H.c.}) + \frac{U}{2} \sum_i (n_i - N)^2, \quad (1)$$

where t is the nearest neighbor hopping integral ($t = 1$ below); U is the on-site repulsion; α is the spin index running from 1 to $2N$; $n_i = \sum_{\alpha=1}^{2N} n_{i\alpha}$ is the total fermion number operator on site i. Equation (1) possesses the particle-hole symmetry $c_{i\alpha} \to (-1)^i c_{i\alpha}^{\dagger}$, which means that it is at half filling. In this case, it is well-known that Eq. (1) is free of the sign problem for all the values of N.

We employ the projector QMC method to investigate its quantum magnetic properties in the ground states. In QMC studies, the long-range ordering is usually obtained through the finite-size scaling of the corresponding structural factors, or, correlation functions. Assuming that the system size is $L \times L$, the extrapolated values as $L \to \infty$ are proportional to the magnitude square of order parameters. Thus it is difficult to distinguish the weakly ordered states from the truly disordered ones. For this reason, there has been a debate whether a quantum spin liquid phase exists near the Mott transition in the honeycomb lattice [40–44]. To overcome this difficulty, we use the pinning-field method [39,44], and measure the spatial decay of the induced order parameters. Order parameters instead of their magnitude square are measured, and thus numerically they are more sensitive to weak orderings. This method has also been used in the projector QMC method recently [44]. To decouple the interaction term, we adopt the Hubbard-Stratonovich transformation in the density channel, which involves complex numbers [45]. We have designed a new discrete Hubbard-Stratonovich decomposition that is exact for the cases from SU(2) to SU(6) Hubbard models, and the algorithm details can be found in the Supplemental Material [46]. Unless specifically stated, the following parameters are used in simulations: the projection time $\beta = 240$ and the discretized imaginary time step $\Delta\tau = 0.05$.

Next we use the pinning-field method to study the magnetic long-range order of the SU$(2N)$ Hubbard model. We define the SU$(2N)$ generators as $S_i^{\alpha\beta} = c_{i,\alpha}^{\dagger} c_{i,\beta} - (\delta^{\alpha\beta}/2N) n_i$. At half filling, in the Heisenberg limit in which charge fluctuations are neglected, each site belongs to the self-conjugate representation with one column of N boxes. Without loss of generality, the classic Néel state configuration can be chosen as follows: each site in sublattice A is filled with N fermions from components 1 to N, while that in sublattice B is filled with components from $N+1$ to $2N$. We define the magnetic moment operator on each site i as

$$m_i = \frac{1}{2N} \left\{ \sum_{\alpha=1}^{N} S_i^{\alpha\alpha} - \sum_{\alpha=N+1}^{2N} S_i^{\alpha\alpha} \right\}. \quad (2)$$

For the configuration defined above, the value of the classic Néel moment is $m_i = (-1)^i \frac{1}{2}$. Within the zero temperature projector QMC method, good quantum numbers are conserved during the projection. Thus we use a pair of pinning fields on two neighboring sites with a Néel configuration to maintain the relation $\langle G | \sum_i S_i^{\alpha\alpha} | G \rangle = 0$ for every α. The pinning-field Hamiltonian is

$$H_{\text{pin},n} = 2N h_{i_0 j_0} \{ m_{i_0} - m_{j_0} \}, \quad (3)$$

where i_0 and j_0 are two neighboring sites defined as $i_0 = (1,1)$ and $j_0 = (2,1)$, respectively. The initial trial wave functions can be chosen as the half-filled plane-wave states. The Hamiltonian Eq. (1) plus Eq. (3) remains free of the sign problem at half filling.

Because the pinning fields in Eq. (2) break the SU$(2N)$ symmetry, the induced magnetic moments prefer the direction defined in Eq. (2). The distribution of m_i is staggered with decaying magnitudes as away from two pinned sites i_0 and j_0. The Néel order parameter is its Fourier component at the wave vector $Q = (\pi, \pi)$ defined as $m_Q(L) = (1/L^2) \sum_i (-1)^i m_i$. The long-range order m_Q can be extrapolated as the limit of

$$m_Q = \lim_{L \to \infty} m_Q(L). \quad (4)$$

This is because the Fourier component of the pinning field at Q is $h_Q = 2h_{i_0 j_0}/L^2$, which goes to zero as $L \to \infty$ for any finite value of $h_{i_0 j_0}$.

To illustrate the sensitivity of the pinning-field method to weak orders, we present the simulations for the SU(6) case of Eq. (1) with $U = 4$. The finite-size scalings of $m_Q(L)$ are presented in Fig. 1 for two different values of $h_{i_0 j_0} = 1$ and 2. Their extrapolated values as $1/L \to 0$ are 0.0261 ± 0.0008 and 0.0253 ± 0.0009, respectively, which are consistent with each other and confirm the validity of this method. Such a small moment is hard to identify using the finite size scaling of the structural factors, as shown in the Supplemental Material [46] and related works [40,42,44]. Another observation is that the induced values of $m_Q(L)$

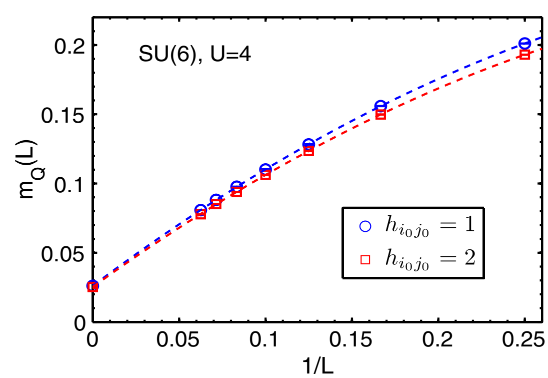

FIG. 1 (color online). Finite size scaling of the residual Néel moment $m_Q(L)$ vs $1/L$ under pinning fields described by Eq. (3) with $h_{i_0 j_0} = 1$ and 2. The largest value of L is 16. The quadratic polynomial fitting is used. Error bars are smaller than symbols.

are weaker at $h_{i_0j_0} = 2$ than those at $h_{i_0j_0} = 1$ at finite values of L, which shows nonlinear correlations between the pinning centers and the measured sites. Certainly they converge in the limit of $1/L \to 0$. In the following, we only present the results of $h_{i_0j_0} = 2$.

One may question whether the pinning-field method overestimates the tendency of long-range ordering. In the Supplemental Material [46], we apply it to the 1D SU(2) and SU(4) Hubbard chains at half filling. In the SU(2) case, the ground state is known as a gapless spin liquid, while in the SU(4) case, it is gapped with dimerization. The pinning-field method shows the absence of long-range Néel ordering in both cases and the asymptotic behavior of power-law spin correlations in the case of SU(2). This further confirms the validity of this method.

We further test the validity of the pinning-field method in the extensively studied half-filled SU(2) Hubbard model in the square lattice by the QMC method [47,48]. The long-range Néel ordering we obtained based on the pinning-field method is consistent with that in previous QMC literature based on the finite-size scaling of structure factors. Our results are shown in the Supplemental Material [46]. The long-range Néel ordering appears from weak to strong interactions. The extrapolated values of m_Q increase as U goes up, and begin to saturate around $U = 10$. At $U = 20$, $m_Q = 0.297 \pm 0.002$, which is in a good agreement with the long-range Néel moment 0.3070(3) of the SU(2) Heisenberg model [49]. This behavior is well known [47,48]: as U goes up, charge fluctuations are suppressed, and thus the low energy physics is described by the Heisenberg model.

Next we simulate the SU(4) Hubbard model, and the magnetic ordering is presented in Fig. 2. Similarly to the SU(2) case, long-range Néel ordering appears for all the values of $U \leq 20$. At each value of U, the extrapolated long-range Néel moment m_Q is weaker than that in the SU(2) case, which is a result of the enhanced quantum fluctuations. Moreover, a striking new feature appears: the relation m_Q vs U becomes nonmonotonic as shown in Fig. 4 below. The Néel moment m_Q reaches the maximum around 0.178 ± 0.008 at $U \approx 8$, and then decreases as U further increases. It remains finite with the largest value of $U = 20$ in our simulations. It is not clear whether m_Q is suppressed to zero or not in the limit of $U \to \infty$. A previous QMC simulation on the SU(4) Heisenberg model shows algebraic spin correlations [35]. It would be interesting to further investigate whether the algebraic spin liquid state survives at finite values of U.

With further increases in $2N$, the Néel ordering is more strongly suppressed by quantum spin fluctuations. The finite-size scalings for the SU(6) case at different values of U are presented in Fig. 3. For all the values of $U \leq 14$, we find nonzero Néel ordering by using the quadratic polynomial fitting. The extrapolated Néel moments m_Q vs U for the SU(6) case are plotted in Fig. 4. For comparison, those of the SU(2) and SU(4) are also plotted together. Similar to the SU(4) case, the long-range Néel moments are nonmonotonic, which reach the maximum around $U \approx 10$. Strikingly, the Néel ordering disappears beyond a critical value of U_c, which is estimated as $14 < U_c < 16$.

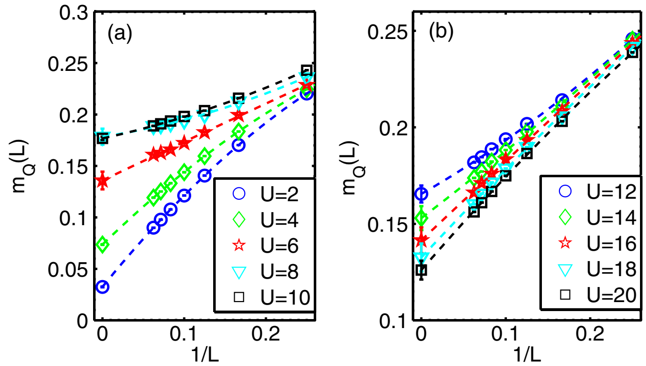

FIG. 2 (color online). Finite size scalings of $m_Q(L)$ vs $1/L$ for the half-filled SU(4) Hubbard model with different values of U. The largest size is $L = 16$. The quadratic polynomial fitting is used. Error bars of QMC data are smaller than symbols.

The low energy effective model of half-filled Hubbard models in the strong-coupling regime is the Heisenberg model. According to the large-N study of the SU($2N$) Heisenberg model with the self-conjugate 1^N representation [27,28], dimerization appears in the large-N limit. Thus the suppression of the Néel order at large values of U is expected from the competing dimer ordering. To investigate this competition, we further apply the pinning-field method to study the dimer ordering for the SU(6) Hubbard model, and the results are presented in Fig. 5. The following dimer pinning field is applied, which changes the hopping integral of a bond i_0j_0 [50],

$$H_{\mathrm{pin,dim}} = -\Delta t_{i_0j_0} \sum_{\alpha} \{c^{\dagger}_{i_0,\alpha} c_{j_0,\alpha} + \mathrm{H.c.}\}, \qquad (5)$$

where i_0 and j_0 are defined as before. The bonding strength between sites i and $i+\hat{x}$ is defined as $d_{i,x} = \frac{1}{2}\langle G|c^{\dagger}_{i\alpha} c_{i+x,\alpha} + \mathrm{H.c.}|G\rangle$, where $|G\rangle$ is the ground

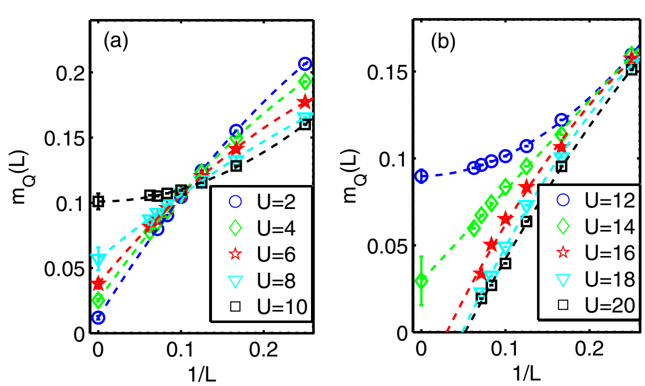

FIG. 3 (color online). Finite size scalings of $m_Q(L)$ vs $1/L$ for the SU(6) Hubbard model at different values of U. The largest size is $L = 16$. The quadratic polynomial fitting is used. Error bars of QMC data are smaller than symbols.

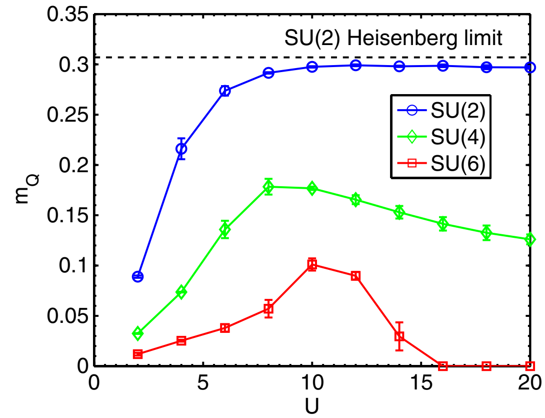

FIG. 4 (color online). The ground state Néel ordering of the 2D half-filled SU($2N$) Hubbard model in the square lattice. The relations of long-range Néel moments m_Q vs U are plotted for $2N = 2$, 4, and 6. For comparison, the SU(2) Heisenberg limit result is plotted as the dotted line. The error bars are obtained from the least square fittings with 95% confidence bounds.

state. We define the dimer order parameter at the wave vector (π, 0) as

$$\dim_{(\pi,0)}(L) = \frac{1}{L^2}\sum_i (-1)^{i_x} d_{i,x}, \qquad (6)$$

where i_x is the x coordinate of site i. Following the same reasoning to extrapolate the long-range Néel ordering as before, we define the long-range dimer order parameter as $\dim_{(\pi,0)} = \lim_{L\to\infty} \dim_Q(L)$. The finite-size scalings for $\dim_{(\pi,0)}(L)$ are plotted in Fig. 5(a), which shows that the columnar dimerization appears when U is above a critical value U_c', which is also estimated around 14–16. It lies in the same interaction regime that Néel ordering starts to vanish. However, whether this transition is of second order such that $U_c = U_c'$ or it is of first order still needs further numeric investigation. We also measure the dimerization at $Q = (\pi, \pi)$ induced by the pinning-field Eq. (5), defined as $\dim_{(\pi,\pi)}(L) = (1/L^2)\sum_i (-1)^i d_{i,x}$, whose finite-size scaling shows the absence of long-range order.

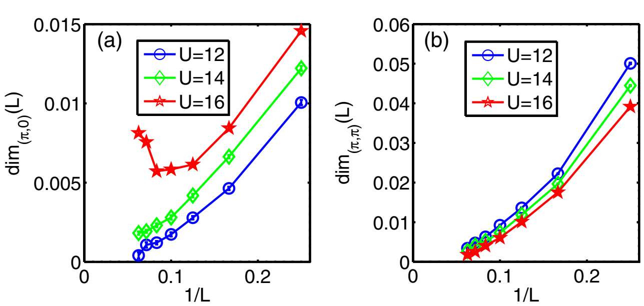

FIG. 5 (color online). Finite-size scalings of the dimer order parameters in the half-filled SU(6) Hubbard model. (a) $\dim_{(\pi,0)}(L)$ and (b) $\dim_{(\pi,\pi)}(L)$ at wave vectors $Q' = (\pi, 0)$ and $Q = (\pi, \pi)$, respectively. The largest size is $L = 16$. Error bars of QMC data are smaller than symbols.

The nature of the transition between the Néel and dimer orderings is an interesting question. In the literature [51,52], ring exchange terms are added to the SU(2) Heisenberg model, which suppress Néel ordering and lead to dimerization. However, our SU(6) case is dramatically different. The SU(6) Néel ordering appears in the regime of weak and intermediate interactions. In this regime ring exchanges are prominent because they reflect short-range charge fluctuations. Our results agree with the picture of Fermi surface nesting because the Néel ordering wave vector $Q = (\pi, \pi)$ is commensurate with the Fermi surface at half filling, while dimerization is not favored because its wave vector $Q' = (\pi, 0)$ does not satisfy the nesting condition [53]. On the other hand, local moment physics dominates when deeply inside the Mott insulating phase in the strong-coupling regime. The exchange energy per site in the dimerized phase is estimated at the order of N^2J with $J = 4t^2/U$, while that of the Néel state is zNJ, where z is the coordination number. Thus dimerization wins when both conditions of large-U and large-N limits are met in agreement with previous theoretical results on SU($2N$) Heisenberg models [27].

Summary.—We have applied the method of local pinning fields in QMC simulations to investigate quantum magnetic properties of the 2D half-filled SU($2N$) Hubbard model in the square lattice. This method is sensitive to weak long-range orders. Long-range Néel ordering is found for the SU(4) case from weak to strong interactions. For the SU(6) case, a transition from the staggered Néel ordering to the columnar dimerization is found as increasing U. The conceivable mechanism is the competition between the weak-coupling Fermi surface nesting physics and the strong-coupling local moment physics. The above QMC simulations may provide a reference point for further investigating the even more challenging problem of doped SU($2N$) Mott insulators.

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