Competing orders in the 2D half-filled SU(2N) Hubbard model through the pinning field quantum Monte-Carlo simulations

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We investigate the ground state magnetic properties of the 2D half-filled SU(2N) Hubbard model in the square lattice by the determinant quantum Monte-Carlo simulations combined with the method of local pinning fields. This method directly gives rise to the values of order parameters instead of their magnitude square, thus it is more accurate at weak orderings than methods using correlation functions. Antiferromagnetic long-range orders are found for both the SU(4) and SU(6) cases at small and intermediate values of \( U \). As increasing \( U \), the long-range Neel moments first grow and then drop. This is very different from the SU(2) case in which the Neel moments increase monotonically and saturate. In the SU(6) case, a transition to the columnar dimer state is found in the strong interaction regime.

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The ultra-cold atom systems have opened up a wonderful opportunity for studying novel phenomena not easily accessible in usual solid state systems. For example, the large-spin ultra-cold alkali and alkaline-earth 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 an object with a large spin \( S \). However, such systems usually only possess the SU(2) symmetry. The leading order magnetic 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 spin ultra-cold fermion systems can possess high symmetries of SU(2N) and Sp(2N). For the simplest case of spin-\( \frac{1}{2} \), a generic Sp(4) symmetry was proved without fine-tuning, which includes the SU(4) symmetry as a special case [2]. Effects from such a high symmetry give rise to exotic properties in quantum magnetism and pairing superfluidity [3–11]. Furthermore, large spin alkaline-earth fermion systems have been experimentally realized in recent years [12–14]. In particular, an SU(6) Mott insulator of \(^{173}\)Yb has also been observed [1, 15]. The above theoretical and experimental progress has stimulated a great deal of interests in the community in exploring novel properties of strongly correlated systems with high symmetries [16–20].

The SU(2N) Heisenberg model was first investigated in the area of condensed matter physics with the purpose to use the large-\( N \) technique to systematically handle strong correlation effects in the context of the study of high \( T_c \) cuprates [21–25]. Mathematically, the SU(2N) spin is expressed by the Young tableau. In a bipartite lattice, the two sublattices can realize two different representations of the SU(2N) group which are complex conjugate to each other. Heisenberg models with such representations have been investigated by the large-\( N \) method [24, 25] and quantum Monte Carlo (QMC) simulations [26–29]. As increasing \( 2N \), enhanced quantum fluctuations have been observed to suppress antiferromagnetic (AF) Neel orderings. For the self-conjugate representations, which corresponds to the half-filled condition for the SU(2N) Hubbard model, consensus has not been achieved yet. In a variational Monte Carlo study on the Heisenberg model with the self-conjugate representations [30], it was found that Neel ordering appear at \( 2N = 2 \) and \( 4 \), and the columnar dimer ordering at \( 2N \geq 6 \). In a determinate QMC work on the \( t-J-U \) model [31], the dimer ordering was found at \( 2N \geq 6 \) in agreement with the variational QMC study, while for the SU(4) case, neither Neel nor dimer ordering exists in the Heisenberg limit. Another open problem is that these previous studies only focus on the Heisenberg limit in which charge fluctuations are completely frozen. It is not clear whether these results are valid in the weak and intermediate values of Hubbard \( U \).

In this article, we perform a systematic DQMC study on the half-filled SU(2N) Hubbard model in the 2D square lattice. The ground state magnetic properties are investigated in both the weak and strong interaction regimes. Instead of measuring correlation functions, we use the local pinning field method and measure the spatial decay of the induced order parameters. The finite-size scaling within this method directly yields the order parameters not the squares of their magnitudes. This method is particularly sensitive to weak ordering as shown in our simulations. We find that long range Neel ordering appears at weak and intermediate values of \( U \) for all the cases we studied from SU(2) to SU(6). For the cases of SU(4) and SU(6), the Neel order is weakened with increasing \( U \). Furthermore, a transition from the Neel state into a columnar dimer ordering phase is observed at a large value of \( U \) in the SU(6) case.
We consider the SU(2N) Hubbard model in the 2D square lattice with the periodic boundary condition as

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

where \( t \) is the nearest neighbor hopping integral scaled to be 1 below; \( U \) is the on-site repulsion; \( \alpha \) 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 \( i \). Eq. 1 possesses the particle-hole symmetry \( c_{i \alpha} \rightarrow (-)^i c_{i \alpha}^\dagger \), which means it is at half-filling. In this case, Eq. 1 is well-known to be free of the QMC sign problem for all the values of \( N \).

We employ the projector QMC to investigate its quantum magnetic properties in the ground states. In most previous QMC studies, the long-range ordering is obtained through the finite size scaling of the corresponding structural factors, or, the two-point correlation functions. However, the extrapolated values as \( 1/L \rightarrow \infty \) are proportional to the magnitude square of order parameters. Thus it is difficult to distinguish the weakly ordered states from the truly disordered ones. Due to this reason, there has been a debate whether a quantum spin liquid phase exists near the Mott transition in the honeycomb lattice [32–36]. To overcome this difficulty, we use the pinning field method [36, 37], and measure the spatial decay of the induced order parameters. Order parameters instead of their magnitude square are measured, and thus numerically it is more sensitive to weak orders. This method has also been used in the project QMC recently [36]. To decouple the interaction term, we adopt the discrete Hubbard-Stratonovich transformation in density channel which involves complex numbers [20, 38, 39]. The parameters used in simulations are the projection time \( \beta = 40 \) and the discretized imaginary time step \( \Delta \tau = 0.05 \).

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

\[ m_i = \frac{1}{2N} \left\{ \sum_{\alpha=1}^{N} S_i^{\alpha \alpha} - \sum_{\alpha=N+1}^{2N} S_i^{\alpha \alpha} \right\}. \tag{2} \]

For the configuration defined above, the value of the classic Neel moment is \( m_i = (-)^i \frac{1}{2} \). For the finite temperature determinant QMC, since the partition function covers all the states in the Hilbert space, we only need to apply the pinning field on a single site. However, in the zero temperature projector QMC method, the good quantum numbers are conserved during the projection. We use a pair of pinning fields on two neighboring sites with a Neel configuration

\[ H_{\text{pin}, n} = h_{ij0} \{ m_{i0} - m_{j0} \}, \tag{3} \]

where sites \( i_0 \) and \( j_0 \) are two neighboring sites \((1,1)\) and \((2,1)\), respectively. The ground states with this configuration of pinning fields are still remain in the sector of \( \langle \sum_i S_i^{\alpha \alpha} \rangle = 0 \) for every \( \alpha \), such that the initial trial wavefunctions can be chosen as the half-filed plane-wave states. The Hamiltonians 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 Neel moment prefers the configuration defined in Eq. 2. The distribution of \( m_i \) is staggered with decaying magnitudes as away from two pinned sites \( i_0 = (1,1) \) and \( j_0 = (2,1) \). The weakest moments are located at the central points \((\frac{3}{2} + \frac{1}{2}, \frac{1}{2} + 1)\) and \((\frac{3}{2} + 2, \frac{1}{2} + 1)\). The residual values at these two points are denoted as \( \pm m(L) \). The moment of the long-range ordering can be extrapolated through as the limit of \( m(L) \) as \( L \rightarrow \infty \). To see this, recall the definition of the long-range-ordered Neel moment as

\[ m_Q = \lim_{h_Q \rightarrow 0} \lim_{L \rightarrow \infty} m_L(h_Q), \tag{4} \]

where \( Q = (\pi, \pi) \); \( h_Q \) is the Fourier component of the external field at the wavevector \( Q \); \( m_L(h_Q) \) is the average Neel moment with \( h_Q \) and the system size \( L \times L \). For the pinning field configuration in Eq. 3, \( h_Q = 2h_{ij0}/L^2 \) goes to zero as \( L \rightarrow \infty \) independent of the value of \( h_{ij0} \). And \( m_Q \) is equivalent to \( m(L \rightarrow \infty) \).

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 the parameter values of \( U = 4 \). The
finite size scaling of $m(L)$ is presented in Fig. 1 for two different values of $h_{i\neq j_0} = 1$ and 2. The extrapolations as $1/L \to 0$ converge to nearly the same value of 0.022 for both $h_{i\neq j_0} = 1$ and 2, which confirms the validity of this method. Such a small moment is beyond the resolution limit of the finite size scaling of the structural factors. One may worry whether the pinning field method overestimates the tendency of long-range ordering. In the supplementary material, 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 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 Neel ordering in both cases and the asymptotic behavior of power-law spin correlations in the SU(2) case. This also confirms the validity of the method. Another point is that the induced values of $m(L)$ are weaker at $h_{i\neq j_0} = 2$ than those at $h_{i\neq j_0} = 1$, although they converge in the limit of $1/L \to 0$. Since the values of $h_{i\neq j_0}$ are finite, this may be a non-linear effect around the pinned sites which disappears as $L \to \infty$. In the following, we only present the results of $h_{i\neq j_0} = 2$.

Next we systematically apply the pinning field method to the SU(2N) Hubbard model in the 2D square lattice of Eq. 1. As a further test of the method, we start with the SU(2) case and present the simulation results in Fig. 2. The long-range ordering of the SU(2) case has been extensively investigated before by performing the finite-size scaling of structure form factors [40, 41]. The results from the pinning field method are consistent with previous studies. The long-range Neel ordering is found from weak to strong interactions. The extrapolated values of $m(L = \infty)$ increase as $U$ goes up, and begin to saturate around $U \geq 10$ to the value $m(L = \infty) \approx 0.29$, which is in a good agreement with the large-Neel moment 0.307 of the SU(2) Heisenberg model [42]. This behavior is well-known [40, 41]: as $U$ goes up, charge fluctuations are suppressed, and the low energy physics is described by the Heisenberg model. The slight decrease of $m(L = \infty)$ as $U$ keeps going up to around 20 is the numerical artifact caused by the finite projection time $\beta$.

We continue to study the magnetic orderings of the SU(4) Hubbard model as presented in Fig. 3. Similarly to the SU(2) case, for all the values of $U$ simulated less than 20, long-range Neel ordering is found. At each value of $U$, the extrapolated long-range Neel moment $m(\infty)$ is weaker than that in the SU(2) case as a result of the enhanced quantum fluctuations. However, a striking difference is the non-monotonic behavior of $m(\infty)$ with increasing $U$. It reaches the maximum around 0.17 at $U \approx 8$, and then decreases with further increasing $U$. The Neel moment $m(\infty)$ remains finite with the largest value of $U = 20$ that we can simulate. In order to infer the behavior of $m(\infty)$ in the Heisenberg limit, i.e., $U \to +\infty$, we replot $m(\infty)$ v.s. 1/$U$ in Fig. 4 (b). It extrapolates to zero before indicating no long-range Neel ordering in the Heisenberg limit. A previous QMC simulation on the SU(4) Heisenberg model shows algebraic spin correlations [31]. It would be interesting to further investigate whether the algebraic spin liquid state survives at finite values of $U$.

As further increasing 2N, the Neel ordering is even more strongly suppressed by quantum fluctuations. The finite-size scalings for the SU(6) case with different values of $U$ are presented in the supplementary material. As $1/L \to 0$, the extrapolated Neel moment $m(\infty)$ v.s. $U$ for the SU(6) case are plotted in Fig. 4 (a). For comparison, those of the SU(2) and SU(4) are also plotted together. Similarly to the SU(4) case, the long-range Neel moments are non-monotonic which reach the maximum around $U \approx 10$. Moreover, the Neel ordering disappears beyond the value of $U_c$ with $U_c \approx 16$. According to the large-$N$ study of SU(2N) Heisenberg model with the self-conjugate $1^N$ representation [24, 25], dimerization appears in the large-$N$ limit. Thus the suppression of the Neel ordering at large values of $U$ is expected to arise from the competition with dimerization.

To investigate the competition between the Neel ordering and dimerization, we further apply the pinning field method to the dimer ordering for the SU(6) Hub-
The magnetic phase diagram for the ground states of the 2D half-filled SU(2N) Hubbard model in the square lattice. The relations of long-range Neel moments $m(\infty)$ v.s. $U$ are plotted for $2N = 2, 4$ and $6$. (b) The data of SU(4) is re-plotted as a function of $1/U$ and fitted with a quadratic polynomial.

The columnar dimer ordering in the half-filled SU(6) Hubbard model. The pinning field $\Delta t_{i,j,0} = 2$ in Eq. 5. Finite size scalings of (a) $\text{dim}_x(L)$ and (b) $\text{dim}_y(L)$ with $1/L$ for different values of $U$. The inset of (b) is the spatial distributions of $d_{x,x}$ with the parameter values $U = 20$ and $L = 12$.

The nature of the transition between the Neel and dimer orderings remains an open question. In previous studies on the SU(2) spin modes [43, 44], ring exchange terms enhance magnetic quantum fluctuations and leads to the transition from Neel to dimer states. However, ring exchanges are of higher order perturbation processes than the bilinear Heisenberg one, and thus are more prominent on the side of weaker $U$. Our SU(6) case is dramatically different since Neel ordering appears at weak interactions. This is natural since the susceptibility of the Neel ordering with the wavevector $Q = (\pi, \pi)$ diverges at half-filling due to Fermi surface nesting even with weak interactions. The dimer ordering occurs at $Q' = (\pi, 0)$ which does not match the nesting condition. It dominates in the Heisenberg limit when deeply inside the Mott insulating states. Whether this transition is of first order or the second order needs further numeric investigation.

In summary, we have shown that the method of the local pinning fields in QMC simulations is more sensitive to detect weak long-range orderings than using structural factors or correlation functions. We apply it to investigate the quantum magnetic properties of the 2D half-filled SU(2N) Hubbard model in the square lattice. Long-range Neel ordering is found for the SU(4) case from weak to strong interactions. For the SU(6) case, a transition from the staggered Neel ordering to the columnar dimerization is found as increasing $U$.

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[1] C. Wu, Nat Phys 8, 784 (2012).
[2] C. Wu, J.-p. Hu, and S.-c. Zhang, Phys. Rev. Lett. 91, 186402 (2003); C. Wu, Modern Physics Letters B 20, 1707 (2006).
[3] C. Wu, Phys. Rev. Lett. 95, 266404 (2005).
[4] K. Hattori, Journal of the Physical Society of Japan 74,
5

3135 (2005).

[5] P. Lecheminant, E. Boulat, and P. Azaria, Phys. Rev. Lett. 95, 240402 (2005).

[6] D. Controzzi and A. M. Tsvelik, Phys. Rev. Lett. 96, 097205 (2006).

[7] M. A. Cazalilla, A. F. Ho, and M. Ueda, New Journal of Physics 11, 103033 (2009).

[8] C. Wu, J. Hu, and S.-C. Zhang, International Journal of Modern Physics B 24, 311 (2010).

[9] P. Corboz, A. M. Lau"{e}hli, K. Penc, M. Troyer, and F. Mila, Phys. Rev. Lett. 107, 215301 (2011).

[10] K. Rodr'iguez, A. Arg"uelles, M. Colom'e-Tatch'e, T. Vekua, and L. Santos, Phys. Rev. Lett. 105, 050402 (2010).

[11] H.-H. Hung, Y. Wang, and C. Wu, Phys. Rev. B 84, 054406 (2011).

[12] B. J. DeSalvo, M. Yan, P. G. Mickelson, Y. N. Martinez de Escobar, and T. C. Killian, Phys. Rev. Lett. 105, 030402 (2010).

[13] S. Taie, Y. Takasu, S. Sugawa, R. Yamazaki, T. Tsutsumoto, R. Murakami, and Y. Takahashi, Phys. Rev. Lett. 105, 190401 (2010).

[14] J. S. Krauser, J. Heinze, N. Flaschner, S. Gotze, O. J"orgensen, D.-S. Luhmann, C. Becker, and K. Sengstock, Nat Phys 8, 813 (2012).

[15] S. Taie, R. Yamazaki, S. Sugawa, and Y. Takahashi, Nat Phys 8, 825 (2012).

[16] M. Hermele, V. Gurarie, and A. M. Rey, Phys. Rev. Lett. 103, 135301 (2009).

[17] A. V. Gorshkov, M. Hermele, V. Gurarie, C. Xu, P. S. Julienne, J. Ye, P. Zoller, E. Demler, M. D. Lukin, and A. M. Rey, Nat Phys 6, 289 (2010).

[18] Z. Cai, H.-h. Hung, L. Wang, D. Zheng, and C. Wu, ArXiv e-prints (2012), arXiv:1202.6323 [cond-mat.quant-gas].

[19] L. Messio and F. Mila, Phys. Rev. Lett. 109, 205306 (2012).

[20] Z. Cai, H.-H. Hung, L. Wang, and C. Wu, ArXiv e-prints (2012), arXiv:1207.6843 [cond-mat.str-el].

[21] I. Affleck, Phys. Rev. Lett. 54, 966 (1985).

[22] D. P. Arovas and A. Auerbach, Phys. Rev. B 38, 316 (1988).

[23] I. Affleck and J. B. Marston, Phys. Rev. B 37, 3774 (1988).

[24] N. Read and S. Sachdev, Nuclear Physics B 316, 609 (1989).

[25] N. Read and S. Sachdev, Phys. Rev. Lett. 62, 1694 (1989).

[26] K. Harada, N. Kawashima, and M. Troyer, Phys. Rev. Lett. 90, 117203 (2003).

[27] N. Kawashima and Y. Tanabe, Phys. Rev. Lett. 98, 057202 (2007).

[28] K. S. D. Beach, F. Alet, M. Mambrini, and S. Capponi, Phys. Rev. B 80, 184401 (2009).

[29] R. K. Kaul and A. W. Sandvik, Phys. Rev. Lett. 108, 137201 (2012).

[30] A. Paramekanti and J. B. Marston, Journal of Physics: Condensed Matter 19, 125215 (2007).

[31] F. F. Assaad and I. F. Herbut, ArXiv e-prints (2013), arXiv:1304.6340 [cond-mat.str-el].

[32] S. R. Hassan and D. Senechal, Phys. Rev. Lett. 110, 096402 (2013).

[33] F. F. Assaad and I. F. Herbut, ArXiv e-prints (2013), arXiv:1304.6340 [cond-mat.str-el].

[34] S. R. Hassan and D. Senechal, Phys. Rev. Lett. 110, 096402 (2013).

[35] F. F. Assaad, eprint arXiv:cond-mat/9806307 (1998), arXiv:cond-mat/9806307.

[36] S. R. White and A. L. Chernyshev, Phys. Rev. Lett. 99, 127004 (2007); F. F. Assaad, in KITP Conference: Exotic Phases of Frustrated Magnets (2012).

[37] J. E. Hirsch, Phys. Rev. B 28, 4059 (1983).

[38] J. E. Hirsch, Phys. Rev. B 31, 4403 (1985).

[39] C. N. Varney, C.-R. Lee, Z. J. Bai, S. Chiesa, M. Jarrell, and R. T. Scalettar, Phys. Rev. B 80, 075116 (2009).

[40] A. W. Sandvik, Phys. Rev. B 56, 11678 (1997).

[41] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Science 303, 1490 (2004).

[42] A. W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007).

[43] F. F. Assaad and H. G. Evertz, “Computational many-particle physics,” (2008).

[44] H. J. Schulz, Phys. Rev. Lett. 64, 2831 (1990).

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Supplementary Material

Projector quantum Monte Carlo and Hubbard-Stratonovich decomposition

We adopt the determinant projector QMC method [45] to study the half-filled SU(2N) Hubbard model. The basic idea is to project a trial wave function |ΨT⟩ using the projection operator e^{−βH}. If |ΨT⟩ is non-orthogonal to the true ground state |ΨG⟩ and a nonzero gap exists between the ground state and the first excited state, the ground state is arrived as the projection time β → ∞,

|ΨG⟩ = \lim_{β→∞} e^{−βH}|ΨT⟩. \tag{7}

The projection time β can be divided into M slices with β = MΔτ.

The second order Suzuki-Trotter decomposition is used to separate the kinetic and interaction energy parts in each time slice,

\[ e^{−Δτ(K+V)} = e^{−ΔτK/2}e^{−ΔτV}e^{−ΔτK/2} + O((Δτ)^3), \tag{8} \]

where K and V represent the kinetic and interaction terms, respectively. For the V term, we can use the discrete Hubbard-Stratonovich (HS) transformation [38] in the density channel to decompose it to the quadratic form

\[ e^{-λ^2(n_i−N)^2} = \frac{1}{4} \sum_{l=±1,±2} γ_i(l)e^{iη_i(l)(n_i−N)} + O(Δτ^4). \tag{9} \]

where \( n_i = \sum_{α=1}^{2N} c_α^+c_α \), γ’s and η’s are discrete HS fields with the following values [39]

\[ γ(±1) = 1 + \frac{\sqrt{6}}{3}, \quad γ(±2) = 1 - \frac{\sqrt{6}}{3}, \]
\[ η(±1) = ±\sqrt{ΔτU(3−\sqrt{6})}, \]
\[ η(±2) = ±\sqrt{ΔτU(3+\sqrt{6})}. \tag{10} \]

After integrating out fermions, we arrive at the fermion determinant whose value depends on the discrete HS fields. The HS fields are sampled using the standard Monte Carlo technique.

The decomposition of Eq. 10 is valid when operator \( n − N \) has any eigenvalues, hence widely used in real calculations [3, 39]. However, we should be careful at large values of \( U \) and \( |n−N| \). In Fig. 6, we plot the values of the left and right hand sides of Eq. 10 as functions of \( ∆τU \) for comparison. We consider the situations of \( |n−N|=1, 2 \) and 3, respectively. The errors of this discrete HS decomposition Eq. 10 depend on \( |n−N| \) significantly. At \( |n−N|=1 \) and 2, the decomposition yields values exact, or, with slight deviations for \( ∆τU < 1 \). However, at \( |n−N|=3 \), the deviation becomes manifest when \( ∆τU > 0.5 \), and even more terribly, the weight becomes negative!

Therefore, we design an exact HS decomposition for the cases from SU(2) to SU(6) in which the operator \( n_i−N \) only takes eigenvalues among \( 0,±1,±2, \) and \( ±3. \) The form of the new HS decomposition is the same as Eq. 10 but it is exact. The values of the discrete HS fields are defined as follows

\[ γ(±1) = \frac{−a(3+a^2)+d}{d}, \quad γ(±2) = \frac{a(3+a^2)+d}{d}, \]
\[ η(±1) = ±\cos^{-1}\left\{\frac{a+2a^3+a^5+(a^2-1)d}{4}\right\}, \]
\[ η(±2) = ±\cos^{-1}\left\{\frac{a+2a^3+a^5-(a^2-1)d}{4}\right\}. \tag{11} \]

where \( a = e^{−ΔτU}, \quad d = \sqrt{8+2a^2(3+a^2)^2} \). This decomposition is used for the simulation of the SU(6) Hubbard model with \( U \geq 10 \) in the main text.

Applications to the 1D SU(2) and SU(4) Hubbard models

As a test to the pinning field method, we apply it to 1D systems whose ground state properties are known. Both the 1D SU(2) and SU(4) Hubbard chains at half-filling will be considered. Below, we present numeric simulations from QMC with pinning fields. The agreement with previous analytic and numeric results confirms the validity of the pinning field method. We use the pinning fields described in the Eq. 3 and Eq. 5 to investigate Neel and dimer orderings, respectively. The pinned sites are fixed as \( i_0 = 1 \) and \( j_0 = 2 \), respectively, and values of the pinning fields are set as \( h_{i_0,j_0} = 2 \) and \( Δτ_{i_0,j_0} = 2 \).

For the 1D half-filled SU(2) Hubbard model, it is well-known that strong quantum fluctuations suppress the long-range Neel ordering. The asymptotic behavior of
the two-point spin correlation functions at half-filling follow the pow-law decay \([46]\)

\[
\langle S(i)S(j) \rangle \sim (-1)^{i-j}\frac{\log L}{|i-j|}.
\]

(12)

Since spin moments are pinned at \(i_0\) and \(j_0\), \(m(L)\) should scale as \((\log L)^{1/4}/L^{1/2}\). Our QMC results with pinning fields are in a good agreement with Eq. 12 as shown in Fig. 7 (a). It is also known that the dimer correlations of the 1D SU(2) Hubbard model exhibit the same asymptotic scaling as that of Eq. 12 [46]. Again, the numeric results agree with this scaling as shown in Fig. 8 (a).

For the 1D half-filled SU(4) Hubbard model, the situation is different. Bosonization analysis [3] shows that its ground states are dimerized with a finite spin gap. Our QMC simulations with pinning fields for the Neel and dimer orderings are illustrated in Fig. 7 (b) and Fig. 8 (b), respectively. Clearly, they show that the Neel-ordering is short-ranged, while the dimerization is long-range-ordered, which agrees with the previous analytic results.

The half-filled SU(6) Hubbard model

In Fig. 9, we present the finite-size scalings for the Neel ordering of the 2D SU(6) Hubbard model. We use the value of the pinning fields \(h_{i_0,j_0} = 2\), and the linear fitting for the data at \(L \geq 8\). The extrapolated long-range Neel moments \(m(\infty)\) for different values of \(U\) are presented in Fig. 4 in the main text.

\[
\begin{array}{ccc}
\text{quantity} & \text{QMC} & \text{ED} \\
\langle m(1,1) \rangle_{U=4} & 0.4338 & 0.4342 \\
\langle m(3,3) \rangle_{U=4} & 0.2354 & 0.2351 \\
\langle m(1,1) \rangle_{U=12} & 0.4797 & 0.4807 \\
\langle m(3,3) \rangle_{U=12} & 0.3204 & 0.3218 \\
\langle m(1,1) \rangle_{U=20} & 0.4902 & 0.4915 \\
\langle m(3,3) \rangle_{U=20} & 0.3241 & 0.3261 \\
\end{array}
\]

TABLE I. Comparison between the QMC and exact diagonalization (ED) results for the half-filled SU(2) Hubbard model. The parameter values are \(h_{i_0,j_0} = 2\), \(\beta = 40\), \(\Delta \tau = 0.05\). The lattice size is \(4 \times 4\).

In order to check the numeric accuracy of our projector QMC simulations, we compare the QMC results for the SU(2) case with those from exact diagonalizations for a small lattice size [47]. Again the pinning fields are applied at sites \(i_0 = (1,1)\) and \(j_0 = (2,1)\) according to Eq. 3 in the main text. In table I, we list the magnetic moments on sites \((1,1)\) and \((3,3)\) with different \(U\)’s. As \(U\) goes up, the numeric errors of QMC increase, but are still less than 0.002 even at \(U = 20\).
However, for large system sizes and high symmetries, exact diagonalizations are no longer applicable. We justify the simulation results by analyzing the errors from the discrete time decomposition $\Delta \tau$ and from the finite projection time $\beta$. From the Suzuki-Trotter decomposition Eq. 8, the error from finite $\Delta \tau$ is at the order $t^2 \Delta \tau^2 U^2$, which is the most severe in the large $U$ limit. Furthermore, the antiferromagnetic exchange energy scale $J$ becomes weaker in this limit, which means that the error from finite $\beta$ is also the worst. Thus in the following, we just present the scaling for the largest value of $U = 20$ in our simulations.

In Fig. 10, we present the scaling of $\Delta \tau$ at $U = 20$. Values of the Neel moment $m(L)$ v.s. $\Delta \tau$ are plotted for the three cases of SU(2), SU(4), and SU(6), respectively. The slopes of the scaling lines are nearly independent on the lattice size $L$ for all three cases. Due to convergence of the finite $\Delta \tau$ scaling, we use the value of $\Delta \tau = 0.05$ for presenting our data.

Next we check the effect of the finite projection time $\beta$. One major conclusion in this paper is the Fig. 4 in the main text which shows the non-monotonic behavior of $m(\infty)$ with increasing $U$ for both the SU(4) and SU(6) cases. Below, we show that this is not an artifact from the finite projection time $\beta$. We have performed calculations with different values of $\beta = 20, 30, 40$ and 60, respectively, for parameter values $U = 20$ and $\Delta \tau = 0.05$. Let us first look at the SU(2) case. After the finite-size scaling v.s. $1/L$, we extrapolate the values of $m(L) = \infty$ at different values of $\beta$ as shown in Fig. 11(a), then the scaling of $m(L = \infty)$ v.s. $1/\beta$ is plotted in Fig. 11(b). It shows that as $\beta \to \infty$, the long-range Neel moment $m(\infty)$ extrapolates to a value 0.302, which is in a good agreement with the QMC result of the SU(2) Heisenberg

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**FIG. 10.** Scaling of the Neel moments $m(L)$ v.s. $\Delta \tau$ for the cases of SU(2), SU(4) and SU(6) shown in (a)–(c), respectively. In the case of SU(2), exact diagonalization results are also plotted as the dotted line for comparison. The parameters are $U = 20$, $\beta = 40$ and $h_{ij,jk} = 2$.

**FIG. 11.** Scalings of the Neel moments $m(L)$ v.s. $1/\beta$ for the SU(4) Hubbard model with $U = 20$. a) The scaling of the Neel moments $m(L)$ v.s. $1/L$ for different values of $\beta$. b) Scaling of the extrapolated value of $m(\infty)$ v.s. $1/\beta$.

**FIG. 12.** Scalings of the Neel moments $m(L)$ v.s. $1/L$ for the SU(6) Hubbard model with $U = 20$. a) The scaling of the Neel moments $m(L)$ v.s. $1/L$ for different values of $\beta$. b) Scaling of the extrapolated value of $m(\infty)$ v.s. $1/\beta$.

**FIG. 13.** The scaling of the Neel moments $m(L)$ v.s. $1/L$ for different values of $\beta$ for the SU(6) Hubbard model with $U = 20$. 

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model. From this extrapolation, we estimate the error of $m(L = \infty)$ at $\beta = 40$ compared with that at $\beta = \infty$ is less than 0.02. In the main text, we use the value of $\beta = 40$ for simulations. Similar scalings are also performed for the SU(4) case as shown in Fig. 12 (a) and (b). Again the result of Neel moments at $\beta = 40$ is very close to the extrapolated value at $\beta = \infty$ with an error less than 0.02. We noticed that in Fig. 4 (a) in the main text, the variations of $m(\infty)$ for both the SU(4) and SU(6) cases are larger than the scale of this error. Therefore, we believe the non-monotonic behavior is not a numeric artifact. At last, let us look at the case of SU(6) are shown in Fig. 13. Different from the above cases, the Neel moments are weakened by increasing $\beta$. Clearly, as $\beta \to \infty$, there is no long-range Neel ordering at $U = 20$.

Combining all the above error analysis, we conclude that our QMC results are reliable.