

# Quantum Monte Carlo simulations of thermodynamic properties of $SU(2N)$ ultracold fermions in optical lattices

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We have systematically studied the thermodynamic properties of a two-dimensional half-filled  $SU(2N)$  Hubbard model on a square lattice by using the determinant quantum Monte Carlo method. The entropy-temperature relation, the isoentropy curve, and the probability distribution of the on-site occupation number are calculated in both  $SU(4)$  and  $SU(6)$  cases, which exhibit prominent features of the Pomeranchuk effect. We analyze these thermodynamic behaviors based on energy scales in the density and spin channels. In the density channel, the interaction strength that marks the crossover from the weak to strong interaction regimes increases with the number of fermion components. In the spin channel, increasing the number of fermion components enhances quantum spin fluctuations, which is shown in the simulations of uniform spin susceptibilities and antiferromagnetic structure factors.

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## I. INTRODUCTION

In condensed matter physics, the goal of generalizing  $SU(2)$  lattice fermion or spin models to those with high symmetries of  $SU(N)$  [1–3] or  $Sp(N)$  [4,5], was originally to employ the systematic  $1/N$  expansion to handle strong correlation physics, especially in the cases with doping or frustrations. Generally speaking, the large symmetries of  $SU(N)$  and  $Sp(N)$  enhance quantum spin fluctuations and suppress the antiferromagnetic (AF) order [1,2,5]. Various exotic quantum paramagnetic phases have been proposed based on the large- $N$  method, including various valence bond solid states and quantum spin liquid states [6–10]. However, in conventional solid states, the  $SU(N)$  symmetry is rare and thus the  $SU(N)$  Hubbard or Heisenberg models are purely of academic interest.

With the rapid development of the ultracold atom experiments, the realization of multicomponent fermionic Hubbard models with the  $SU(2N)$  or  $Sp(2N)$  symmetry has become a realistic goal (the number of fermion components due to the hyperfine spin degree of freedom is naturally an even number). It was proposed that the simplest  $Sp(2N)$  and  $SU(2N)$  Hubbard models with  $2N = 4$  can be realized in the hyperfine spin- $\frac{3}{2}$  alkali and alkaline-earth atoms [11,12]. In these spin- $\frac{3}{2}$  Hubbard models, an exact  $Sp(4)$  spin symmetry exists without any fine tuning of parameters, which is further enlarged to  $SU(4)$  when the interactions do not rely on hyperfine spin. The alkaline-earth atoms, e.g.,  $^{173}\text{Yb}$  and  $^{87}\text{Sr}$ , have a closed shell of valence electrons and thus their hyperfine spins are simply nuclear spins. The interactions between the atoms with different hyperfine spins are insensitive to the nuclear spins, leading to the  $SU(2N)$  symmetry with  $2N$  being the number of fermion components [13,14].

Recently, significant progress has been made in the experiments of ultracold alkaline-earth fermions with large hyperfine spins. The  $^{173}\text{Yb}$  and  $^{87}\text{Sr}$  atoms have been cooled down to quantum degenerate temperatures [15–17], revealing the  $SU(6)$  and  $SU(10)$  symmetries, respectively. Furthermore, an

$SU(6)$  single-band fermionic Hubbard model has also been realized with  $^{173}\text{Yb}$  atoms in a three-dimensional (3D) optical lattice [18]. Beyond the single-band case, the spin-exchange interactions have recently been observed in the two-orbital  $SU(6)$  and  $SU(10)$  fermion system, respectively [19,20]. Moreover, the number of spin components can be tuned experimentally [21]. Theoretically, the novel symmetries of the multicomponent Hubbard model can give rise to the novel superfluidity [22–28] and exotic quantum magnetism [29–38].

In ultracold atom experiments, achieving low enough temperature regime below the spin superexchange scale has been considered a benchmark for simulating strongly correlated quantum systems. Despite numerous efforts by experimentalists, achieving this temperature regime is still out of reach and remains one of the most challenging problems in this field. So far, ultracold fermions in optical lattices have been cooled down to temperature regime below the hopping energy scale,  $T \sim t$ . One of the promising schemes for further cooling the system into spin superexchange scale  $T \sim J$  is known as interaction-induced adiabatic cooling [39], a cooling scheme by adiabatically increasing interactions. This cooling scheme utilizes the Pomeranchuk effect, which was originally proposed in the  $^3\text{He}$  systems. However, for a conventional two-component Hubbard model in lattices, the Pomeranchuk effect is weak due to the antiferromagnetic correlations in the  $SU(2)$  Mott insulator. It is still controversial whether the system can be cooled down to spin superexchange temperature by Pomeranchuk cooling [39–42]. As we show below, the multicomponent  $SU(2N)$  Hubbard model significantly facilitates the Pomeranchuk cooling, cooling the system down to the temperature scale of  $J$  from an initial temperature that is currently accessible in experiments.

This paper extends the previous work reported in Ref. [43]. We have performed detailed determinant quantum Monte Carlo (DQMC) simulations of thermodynamic properties of the half-filled  $SU(2N)$  Hubbard model with  $2N = 4$  and 6 in the temperature regime  $J < T < t$ . We calculated the entropy-temperature relation and isoentropy curves, which show the enhancement of entropy with increasing interaction strength

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in the intermediate temperature regime, i.e., the Pomeranchuk effect. The probability distributions of the on-site occupation number show the enhancement of particle localization as temperature increases in the low and intermediate temperature regimes. The uniform spin susceptibilities and AF structure factors are also calculated.

The rest of this paper is organized as follows. In Sec. II, we introduce the definition of the SU(2N) Hubbard model. A discussion of the density and spin energy scales of the half-filled SU(2N) Hubbard model is followed in Sec. III. The parameters of the DQMC simulations are given in Sec. IV. In Sec. V, we present the results of DQMC study on the thermodynamic properties of the half-filled SU(4) and SU(6) Hubbard models. Subsequently the probability distribution of on-site occupation number is calculated in Sec. VI. In Sec. VII, the magnetic properties at finite temperatures are investigated. Conclusions are drawn in Sec. VIII.

## II. SU(2N) HUBBARD MODEL

Since naturally the number of fermion components due to the hyperfine spin degree of freedom is an even number, we only consider Hubbard model with SU(2N) symmetry. At half-filling, an SU(2N) Hubbard model is defined by the lattice Hamiltonian:

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

where  $\langle i, j \rangle$  denotes nearest neighbors and the sum runs over sites of a two-dimensional square lattice;  $\alpha$  represents spin indices running from 1 to 2N;  $n_i$  is the particle number operator on site  $i$  defined by  $n_i = \sum_{\alpha=1}^{2N} c_{i\alpha}^\dagger c_{i\alpha}$ ;  $t$  and  $U$  are the nearest-neighbor hopping integral and the on-site interaction, respectively.

This definition of Hubbard Hamiltonian Eq. (1) offers several advantages. In the atomic limit ( $t = 0$ ), consider a half-filled lattice with  $N$  particles per site, the energy cost of moving a particle from one site to its neighboring site is  $U$ , which is independent of  $N$ . Due to half-filling, the chemical potential  $\mu$  vanishes in this grand canonical Hamiltonian, and thus is not explicitly shown in Eq. (1). Equation (1) possesses the particle-hole symmetry in bipartite lattices, which removes the sign problem in DQMC simulations for an arbitrary value of  $2N$ .

In terms of the multiplets of SU(2N) fermions in the fundamental representation, the generators of the SU(2N) group can be written as

$$S_{\alpha\beta}(i) = c_{i\alpha}^\dagger(i) c_{i\beta}(i) - \frac{\delta^{\alpha\beta}}{2N} \sum_{\gamma=1}^{2N} c_{i\gamma}^\dagger(i) c_{i\gamma}(i), \quad (2)$$

where  $\alpha$  and  $\beta$  run from 1 to 2N. The generators defined above are not independent of each other, since the diagonal operators satisfy the relation,  $\sum_{\alpha} S_{\alpha\alpha}(i) = 0$ . Nevertheless, the definition of operators, Eq. (2), results in a simple commutation relation

$$[S^{\alpha\beta}, S^{\gamma\delta}] = \delta_{\beta\gamma} S^{\alpha\delta} - \delta_{\alpha\delta} S^{\gamma\beta}. \quad (3)$$

For convenience, we define the structure factor  $S_{su(2N)}(\mathbf{q})$  as

$$S_{su(2N)}(\mathbf{q}) = \frac{1}{L^2} \sum_{i,j} e^{i\mathbf{q}\cdot\mathbf{r}} S_{\text{spin}}(i,j), \quad (4)$$

where  $\mathbf{r}$  is the relative vector between sites  $i$  and  $j$ .  $S_{\text{spin}}(i,j)$  is the SU(2N) version of equal-time spin-spin correlation functions defined by

$$S_{\text{spin}}(i,j) = \frac{1}{(2N)^2 - 1} \sum_{\alpha,\beta} \langle S_{\alpha\beta,i} S_{\beta\alpha,j} \rangle. \quad (5)$$

## III. ENERGY SCALES IN DENSITY AND SPIN CHANNELS

Before going to the results of DQMC simulation, let us present a qualitative understanding of the physics of the half-filled Hubbard model on a square lattice. The density channel and spin channel are characterized by two energy scales  $\Delta_c$  and  $\Delta_s$ , respectively, which will be discussed in both the weak and strong interaction regimes below. In condensed matter literature, the term of charge channel is more frequently used. To avoid confusion, here we use density instead of charge, since ultracold atoms are neutral.

### A. Weak interaction regime and atomic limit

We first consider the weak interaction limit ( $U \rightarrow 0$ ). In this regime, the underlying Fermi surface plays an important role, which possesses the diamond shape and thus exhibits perfect nesting. The key physics then arises from the Fermi surface nesting: the spin susceptibility in the noninteracting limit diverges logarithmically, and thus an infinitesimal repulsive interaction generates the AF long-range order. In this case, the gapped quasiparticle excitations carry both quantum numbers of particle number and spin. The density and spin energy scales are identical in this regime as [44]

$$\Delta_s/t = \Delta_c/t = 4\pi^2 e^{-2\pi\sqrt{t/U}}. \quad (6)$$

Certainly, in the weak interaction regime, the system is a weak insulator. Although it is gapped, density fluctuations cannot be neglected. On the contrary, in the atomic limit ( $t = 0$ , or  $U \rightarrow +\infty$ ), the Fermi surface completely disappears, and we need to use the local moment picture. At zero temperature, density fluctuations are completely frozen. In the Mott-insulating state, we use the single-particle gap to denote the density fluctuations, i.e., the energy cost by adding or removing a particle from the Mott-insulating state. It is the energy difference between the two energy levels  $\Delta_c = E_{n_i=N+1} - E_{n_i=N}$ , which equals  $\frac{U}{2}$  in the atomic limit. Since the hopping process is completely suppressed, the AF exchange energy  $J = 0$ , i.e., the spin energy scale  $\Delta_s$  is zero in the atomic limit.

### B. Strong interaction regime

Let us consider the strong interaction regime in which  $U$  is large but not strong enough to completely suppress density fluctuations, i.e.,  $t/U \ll 1$ . Let us consider the density channel energy scale  $\Delta_c$  by adding an extra particle (hole) onto the background of the Mott-insulating state. As shown in Fig. 1(a), the propagation of the particle (hole) expands the excitation energy level at  $U/2$  in the atomic limit into an energy band. The density channel gap corresponds to the band bottom and thus is lowered to

$$\Delta_c = \frac{U}{2} - \frac{W}{2}, \quad (7)$$

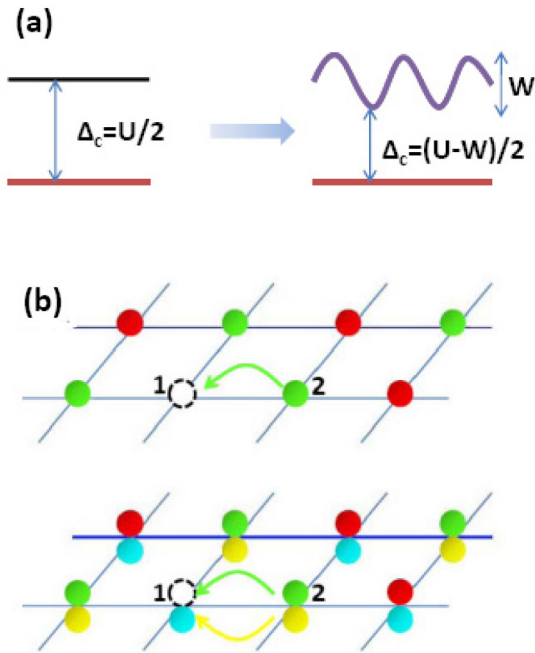


FIG. 1. (Color online) (a) Energy dispersion of a hole excitation on the background of the half-filled Mott-insulating state: (left) the atomic limit with  $t/U = 0$ , (right)  $t/U \ll 1$ . (b) Sketches of a hole hopping in the SU(2) (up) and SU(4) (down) AF backgrounds, respectively. (Figure 1(b) is from Ref. [43].)

where  $W$  is the band width and is determined by the hopping process of the extra particle (hole).

In Fig. 1(b), we compare the hopping process of an extra hole in the half-filled SU(2) and SU(4) Mott insulators. In the SU(4) case, there are many more routes for the hole to hop from one site to its neighboring site than it does in the SU(2) case. Typically speaking, the number of hopping process for an extra particle or hole under the half-filled Mott-insulating background scales as  $N$ , thus we estimate  $W \propto Nt$ . The mobility of the extra hole is greatly enhanced in the SU(2N) Mott-insulating state. Consequently, the density channel energy scale  $\Delta_c$  is significantly lowered with increasing  $2N$ . Naively, we could estimate that  $\Delta_c$  vanishes at

$$U_c \approx Nt. \quad (8)$$

Certainly, due to Fermi surface nesting,  $\Delta_c$  does not vanish even in the weak interaction regime but becomes exponentially small. Nevertheless,  $U_c$  sets up a scale of interaction strength to separate the regime of the Fermi surface nesting and that of local moments.

The low-energy physics in the strong interaction regime is described by the SU(2N) generalization of the Heisenberg model:

$$H = J \sum_{\alpha, \beta, \vec{i}, \vec{j}} S_{\alpha\beta, \vec{i}} \bar{S}_{\beta\alpha, \vec{j}}, \quad (9)$$

where the SU(2N) spin operators are defined in Eq. (2).  $J$  describes the strength of spin superexchange energy scale, which can be viewed as the spin energy scale  $\Delta_s$ . The second-order perturbation theory yields  $J = 4t^2/U$ , which decreases as  $U$  increases. Noting that  $\Delta_s \approx 4\pi^2 t e^{-2\pi\sqrt{t/U}}$  in the weak

interaction regime, which increases with  $U$ , there should exist a peak in the intermediate interaction regime.

### C. Finite-temperature effect

When the fermion system is deep in the Mott-insulating state, in the low-temperature regime  $T \ll \Delta_s$ , density fluctuations are strongly suppressed, and the physics is dominated by the spin superexchange process. Therefore quantum spin fluctuations play an important role in determining the magnetic properties of the Mott-insulating state at low temperatures. On the contrary, at high temperatures  $T \gg \Delta_c$ , quantum fluctuations give way to thermal fluctuations, which suppress quantum correlations, and thus interaction effects can be neglected. In the intermediate temperature regime  $\Delta_s < T < \Delta_c$ ,  $T$  is high enough to suppress the AF correlations, but not sufficient to defreeze the on-site particle number fluctuations. Both quantum and thermal fluctuations are important in the intermediate temperature regime, and the interplay between them gives rise to interesting phenomena and universal properties [45].

## IV. DQMC METHOD

The DQMC method is a widely used nonperturbative method for studying strongly correlated fermion systems [46–53]. Provided that there is no sign problem, DQMC is known to be a well-controlled and unbiased method, which yields asymptotically exact results through finite size scaling. One of the most remarkable DQMC results is the AF long-range order in the ground state of 2D SU(2) half-filled Fermi-Hubbard model on a square lattice [48,49,54]. In the subsequent sections, we will use the DQMC method to simulate the thermodynamic properties of the half-filled SU(2N) Hubbard model in different regimes of temperature  $T$  and interaction  $U$ . We will also show how those results are related to the two energy scales  $\Delta_s$  and  $\Delta_c$  analyzed in previous section.

Considering the error accumulation from matrix multiplications and simulation time, the lowest temperature in simulations is set as  $T_L/t = 0.1$  (with  $\beta = t/T_L = 10$ ). The Suzuki-Trotter decomposition is used in which the error is proportional to the cube of time discretization parameter  $(\Delta\tau)^3$ .  $\Delta\tau$  is set from 0.02 to 0.05 in the temperature regime  $T_L/t < T/t < 0.5$ , and the convergence with respect to the scalings of  $\Delta\tau$  has been checked.

The Hubbard-Stratonovich (HS) transformation in the determinant QMC algorithm can be performed in the density channel [7] preserving the SU(2) symmetry of the Hubbard model, which can also be generalized to the SU(2N) Hubbard model. The discrete HS decomposition with an Ising field only applies to the spin- $\frac{1}{2}$  case [47,48]. For the cases of SU(4) and SU(6), an exact discrete decomposition has been developed in Ref. [55], which is explained in the Appendix and employed in our simulations. The simulated system is a  $L \times L$  square lattice with  $L = 10$ . We focus on the parameter regimes of  $0.1 < T/t < 10$  and  $2 \leq U/t \leq 12$ . For a typical data point, we use 10 QMC bins each of which includes 2000 warm-up steps and 8000 measurement steps. We collect data once in each time slice. In our simulations,  $t$  is set to unity and then the Hubbard  $U$  and temperature  $T$  are given in the unit of  $t$ .

## V. THERMODYNAMIC PROPERTIES OF HALF-FILLED SU(2N) HUBBARD MODEL

In this section, we present the simulations of the thermodynamic properties of the half-filled SU(2N) Hubbard model with  $2N = 4$  and 6 on a square lattice, including the entropy-temperature relation, and the Pomeranchuk effect.

### A. Entropy-temperature relation

In cold atom experiments, entropy is actually a more physical quantity than temperature to characterize the system. Below we present the simulated entropy in the half-filled SU(4) and SU(6) Hubbard models. The parameters of simulation are chosen in the regimes of  $0.1 < T/t < 10$  and  $2 \leq U/t \leq 12$ , which are of interest in experiments. The simulated entropy per particle (not per site) is defined by  $S_{SU(2N)} = S/(NL^2)$ , where  $S$  is the total entropy in the lattice. The following formula is employed to calculate  $S_{SU(2N)}$ :

$$\frac{S_{SU(2N)}(T)}{k_B} = \ln 4 + \frac{E(T)}{T} - \int_T^\infty dT' \frac{E(T')}{T'^2}, \quad (10)$$

where  $\ln 4$  is the entropy at infinite temperature;  $E(T)$  denotes the internal energy per particle at temperature  $T$ .

In Fig. 2, we show the entropy (per particle) of SU(4) and SU(6) fermions as a function of  $T$  for various values of  $U$ . In both cases, the curves cross at two typical temperatures  $T_l$  (low) and  $T_h$  (high), which divide the temperature into three different regimes. Let us first look at the SU(4) case as follows.

*Low-temperature regime*  $T_L < T < T_l$ . In this regime, the dependence of the entropy per particle  $S_{SU(2N)}$  on  $U$  is nonmonotonic, which can be understood by the competition between the spin energy scale  $\Delta_s$  and the density energy scale  $\Delta_c$  as explained below.

For weak interactions  $U/t < 4$ ,  $S_{SU(4)}$  is insensitive to  $U$ . As explained in Sec. III A, the physics in this regime is characterized by the Fermi surface nesting  $\Delta_c$  and  $\Delta_s$  which are equal and are smaller than  $T_L/t \approx 0.1$  (the lowest temperature reached in our simulations), and thus interaction effects are unimportant.  $S_{SU(4)}$  is then approximately the same as that in the noninteracting limit. The nonzero residue entropy is due to the finite-size effect, which is caused by the degeneracy of single-particle states right located on the Fermi surface. As  $U$  increases,  $\Delta_c$  increases faster than  $\Delta_s$ , while  $\Delta_s$  quickly reaches its maximum. In this interaction regime, the relation  $\Delta_c > \Delta_s > T$  holds, and thus increasing  $U$  freezes the on-site particle number fluctuations and enhances AF correlations. Even though there cannot be true long-range AF ordering at finite temperatures in two dimensions, the AF correlation length scales as  $e^{-\frac{2}{U}}$ . Consequently,  $S_{SU(4)}$  drops with increasing  $U$  and the residue entropy, in principle, approaches zero. If  $U$  continues to increase and reaches the strong interaction regime, say,  $U/t > 8$ ,  $\Delta_c \simeq U/2$  increases while  $\Delta_s \simeq J = 4t^2/U$  decreases. Thus the relation  $\Delta_c \gg T \gg \Delta_s$  holds.  $T$  is low enough to freeze the on-site particle number fluctuations but high enough to disorder AF correlations. Therefore, increasing  $U$  (or equivalently, decreasing

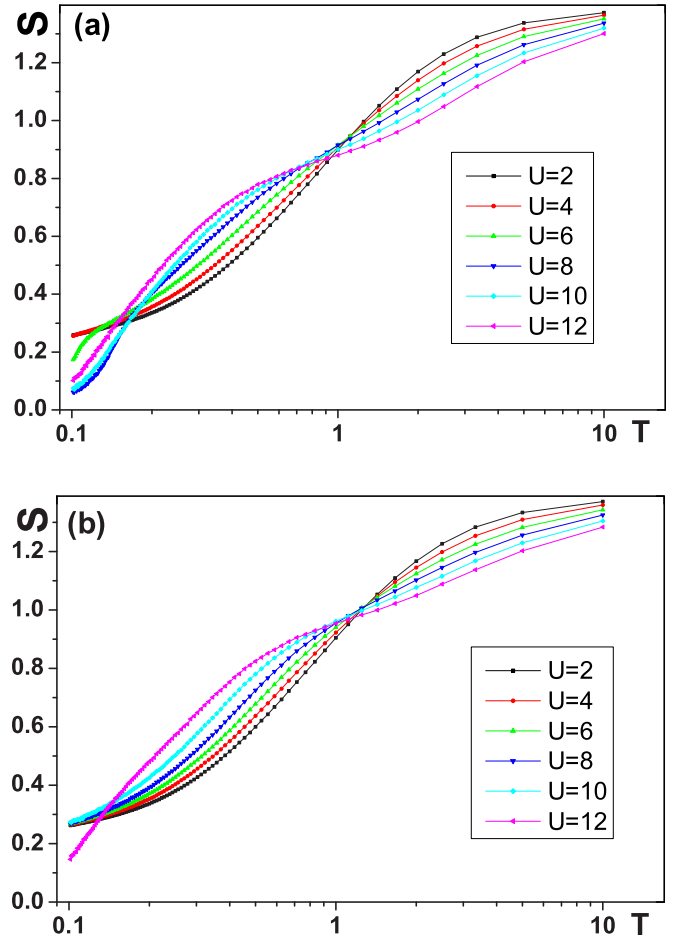


FIG. 2. (Color online) The entropy per particle as a function of  $T$  at different values of  $U$  in (a) SU(4) and (b) SU(6) Hubbard models. The system size is  $L \times L$  with  $L = 10$ .

$\Delta_s$ ) enhances the entropy at a fixed  $T$  in the low temperature regime.

*Intermediate-temperature regime*  $T_l < T < T_h$ . In this temperature regime,  $S_{SU(4)}$  monotonically increases with  $U$  at a fixed  $T$ . At small  $U$  the system is in the weak Mott-insulating state with small values of  $\Delta_s$  and  $\Delta_c$ , which is very close to a Fermi liquid state. The system enters the solidlike strong Mott state at large  $U$ , where the physics is mostly local-moment-like. The increase of entropy with  $U$  means that the liquidlike state is more ordered than the solidlike state, known as the Pomeranchuk effect. In this temperature regime,  $T$  is high enough compared to  $\Delta_s$ , and thus thermal fluctuations suppress magnetic correlations, while it remains smaller than  $\Delta_c$ , such that the on-site particle number fluctuations are still frozen. In the strong Mott-insulating state, fermions on each site are nearly independent of each other, and thus the entropy per site is proportional to the logarithm of the spin degeneracy. In the weak Mott-insulating state, we could think there is still a reminiscence of Fermi surface, which strongly suppresses the entropy contribution. Therefore, the liquidlike state is more ordered than the solidlike state in the intermediate-temperature regime.

On the other hand, the Pomeranchuk effect does not occur in the low-temperature regime ( $T \ll \Delta_s$ ), where thermal



fluctuations are not strong enough to suppress AF correlations. In this case, the AF correlations between adjacent sites lift spin degeneracy and lower the entropy in the strong Mott-insulating state. Consequently, the Pomeranchuk effect is prominent in the intermediate-temperature regime.

*High-temperature regime*  $T > T_h$ . In this case, not only spin fluctuations but also the on-site particle number fluctuations are defrozed by thermal fluctuations  $T > \Delta_c$ . Thus the on-site particle number fluctuations make a significant contribution to the entropy. Therefore, increasing  $U$  can decrease the on-site particle number fluctuations and thus lowers the entropy at a fixed  $T$  in the high temperature regime.

As for the SU(6) case, the behavior of entropy vs  $U$  and  $T$  is qualitatively similar to that in the SU(4) case. Nevertheless, the intermediate temperature regime of the former is broader than the latter, which means that the Pomeranchuk effect is more prominent.

### B. Pomeranchuk effect

As analyzed in Sec. V A, in the strong Mott-insulating regime the lattice system has larger entropy capacity than in the weak Mott-insulating regime, which leads to the Pomeranchuk effect. This effect was first proposed in the  $^3\text{He}$  system, where, in the low-temperature regime, increasing pressure adiabatically can further cool the system. In low-temperature physics, this effect was employed as an effective cooling method named after Pomeranchuk. The similar situation occurs in the Hubbard model. Nevertheless, at low temperatures where the AF correlations are important, the spin degeneracy is lifted, which reduces the entropy in the Mott-insulating state. In this case, the Pomeranchuk effect does not occur. The DQMC simulations have been performed for the half-filled SU(2) Hubbard model in the literature. Both in 2D and 3D cases, the Pomeranchuk effect is not obvious in the range of the entropy per particle  $S_{SU(2)}$  between 0.1–0.9, even if the interaction achieves  $U/t \sim 10$  [40–42].

In the multicomponent SU( $2N$ ) Hubbard model, the situation is different. Due to the increase of the number of fermion components, the Pomeranchuk effect is greatly amplified [43,56]. The isoentropy curves vs  $U$  and  $T$  are plotted in Figs. 3(a) and 3(b) for the SU(4) and SU(6) Hubbard models, respectively. In both cases, the Pomeranchuk effects are prominent in the intermediate-temperature regime with intermediate interaction strengths, which emerge at  $0.4 < S_{SU(4)} < 0.8$  for the SU(4) case, and at  $0.3 < S_{SU(6)} < 0.9$  for the SU(6) case.

The enhancement of the Pomeranchuk effect can be illustrated by comparing the SU(2) and SU(4) cases. When deeply inside the Mott-insulating state, in the intermediate temperature regime, the AF correlations can be neglected, and the entropy per particle  $S_{SU(2N)}$  is dominated by the contribution of spin degeneracy. Therefore, the entropy capacities can be estimated as  $S_{SU(2)} = \ln 2 \approx 0.69$ , which is smaller than  $S_{SU(4)} = \ln C_4^2/2 \approx 0.89$ . On the other hand, in the intermediate interaction regime, the density channel gap in the SU(4) case is significantly smaller than that in the SU(2) case for the same interaction  $U$ . This means that fermions in the SU(4) Hubbard model can be more easily excited to the

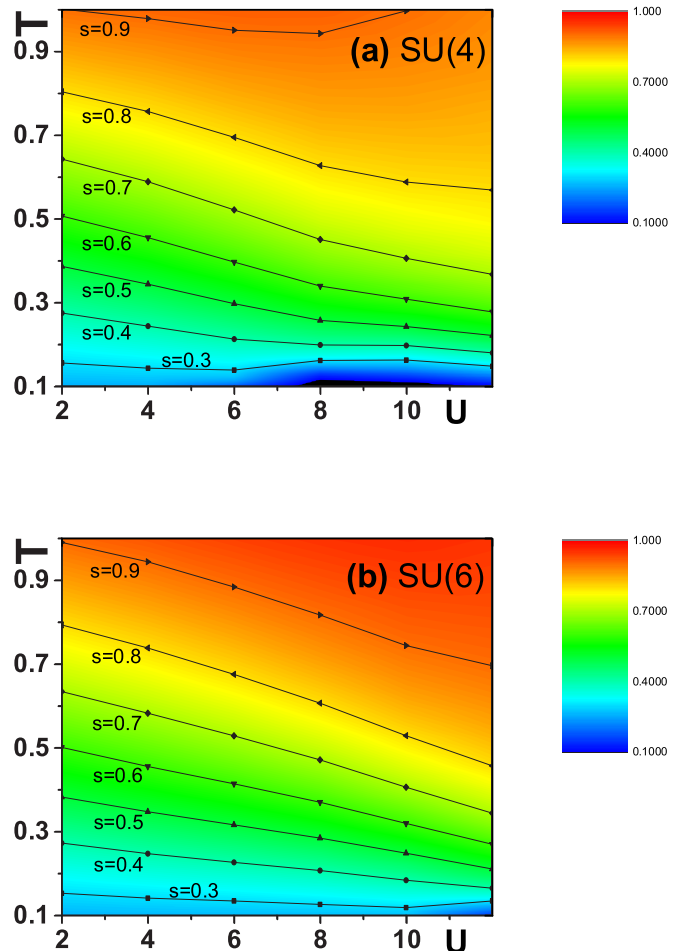


FIG. 3. (Color online) The isoentropy curves for the half-filled (a) SU(4) and (b) SU(6) Hubbard models on a  $10 \times 10$  square lattice. The entropy per particle  $S_{SU(2N)}$  is indicated on each curve. (b) was published in Ref. [43], which is reproduced here with a new curve of  $S_{SU(6)} = 0.3$  added.

upper Hubbard band than those in the SU(2) case, which also enhances the entropy capacity of fermions in the SU(4) case.

### VI. PROBABILITY DISTRIBUTION OF ON-SITE OCCUPATION NUMBER

To characterize the on-site particle number fluctuations, we study the probability distribution of the on-site occupation number. In the SU(2) case, at half filling the double-occupation number  $n_d(i) = \langle n(i)_\uparrow n(i)_\downarrow \rangle$  is related to the local moment  $\langle m_z^2 \rangle = 1 - 2n_d$ , which exhibits a slightly nonmonotonic behavior as a function of  $T$  for fixed  $U$  [57]. Also, in cold atom experiments, this quantity can be measured with *in situ* single-site resolution techniques [58,59]. Let us consider the SU(4) case. At half filling the most probable configuration of on-site particle number is  $n(i) = 2$ . At finite  $U$ , particles are allowed to hop between different sites, leading to on-site particle number fluctuations. Due to the particle-hole symmetry, the probabilities for the occupation numbers  $n$  and  $2N - n$  are equal. Thus we only need to calculate  $P(n)$  with  $n = 0, 1$ , and

2, respectively. They are defined as

$$\begin{aligned}
 P(0) &= \prod_{\alpha=1}^4 (1 - n_i^\alpha); \\
 P(1) &= \sum_{\alpha=1}^4 n_i^\alpha \prod_{\beta \neq \alpha} (1 - n_i^\beta); \\
 P(2) &= \sum_{\alpha \neq \beta} n_i^\alpha n_i^\beta \prod_{\gamma \neq \alpha, \beta} (1 - n_i^\gamma).
 \end{aligned} \tag{11}$$

Obviously, they satisfy the relation  $2P(0) + 2P(1) + P(2) = 1$ .

The simulation results of  $P(n)$  ( $n = 0, 1$  and  $2$ ) as a function of  $T$  for various  $U$  are presented in Fig. 4. In the weak and intermediate interaction regimes, density fluctuations are significant. The maximal probability of the exact half-filling  $P(2)$  only achieves around 70% when  $U/t = 6$ . In contrast, the probabilities of one-particle fluctuation defined by  $2P(1)$  fall in the range between 30% and 40%. The probabilities of two-particle fluctuation,  $2P(0)$ , are typically as low as a few percent. Each  $P(n)$  ( $n = 0, 1$ , and  $2$ ) exhibits nonmonotonic behavior as  $T$  increases. For example, at low temperatures  $P_0$  and  $P_1$  fall with the increase of  $T$ ; then after reaching their minima at the temperature scale around  $t$ , they grow again. This indicates that in the temperature regime  $T < t$ , the on-site particle number fluctuations are suppressed with increasing  $T$ . This counterintuitive phenomenon reminds us of the Pomeranchuk effect, that the system tends to localize fermions in the intermediate temperature regime to maximize the entropy, which mainly comes from the spin degeneracy. When the temperature further increases, the particle number fluctuations are activated and grow with  $T$ .

## VII. MAGNETIC PROPERTIES

In this section, we study the magnetic properties of the half-filled  $SU(2N)$  ( $2N = 4$  and  $6$ ) Hubbard model on a square lattice at finite temperatures, including both the uniform spin susceptibilities and the AF structure factor.

### A. Uniform spin susceptibilities

We now consider the uniform spin susceptibilities  $\chi_{SU(2N)}$ . Because the total spin is conserved,  $\chi_{SU(2N)}$  can be expressed as the equal-time correlations through the structure factor at  $\mathbf{q} = 0$ :

$$\chi_{su(2N)}(T) = \frac{1}{k_B T} S_{SU(2N)}(\mathbf{q} = 0), \tag{12}$$

where the structure factor  $S_{su(2N)}(\mathbf{q})$  is defined by Eq.(4).

In the 2D half-filled  $SU(2)$  Hubbard model [42], or, the Heisenberg model [60], it is known that at high temperatures,  $\chi_{su(2)}$  behaves as the Curie-Weiss law, which is proportional to  $1/T$ . At low temperatures,  $\chi_{su(2)}(T)$  is suppressed due to the AF correlations, and therefore it exhibits a peak at a low-temperature scale  $T_p$ .  $T_p$  can be used to roughly characterize the spin energy scale  $T_p \simeq \Delta_s$  (in Heisenberg model  $T_p \simeq J$ ).

The simulation results of the uniform spin susceptibilities for the  $SU(4)$  and  $SU(6)$  Hubbard models are presented in

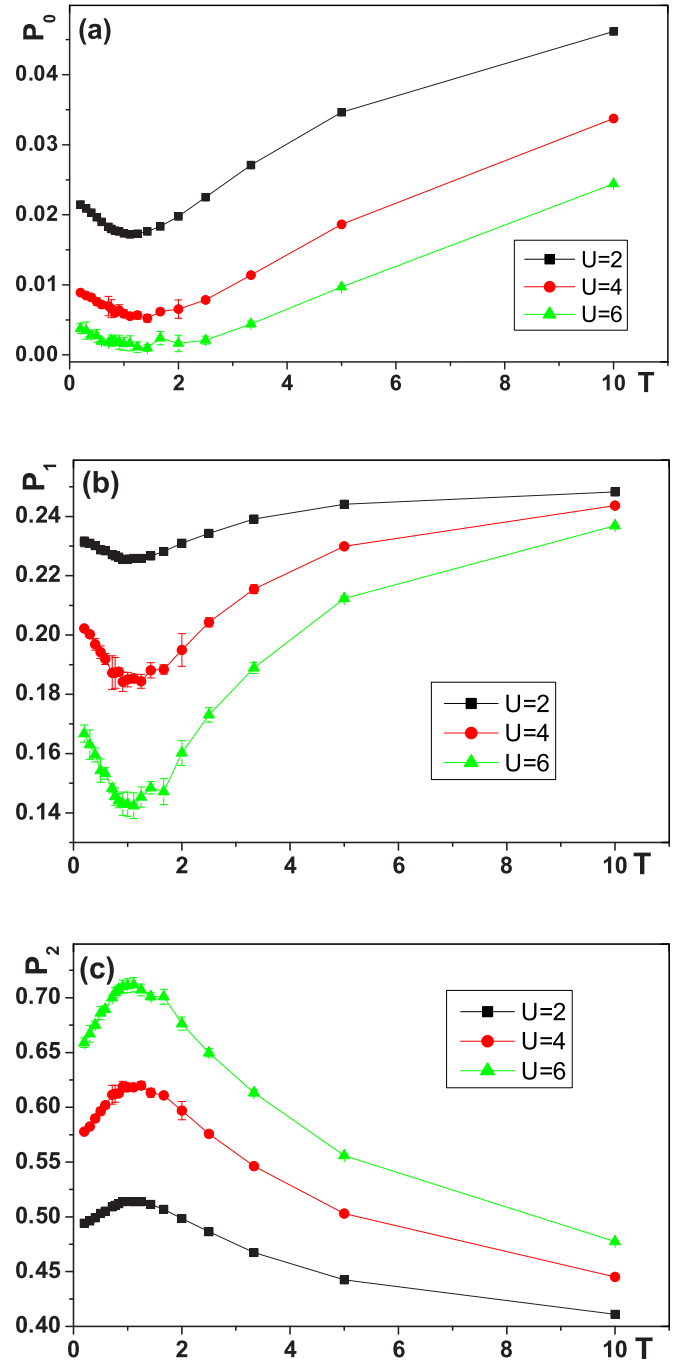


FIG. 4. (Color online) The probabilities  $P(n)$  for the on-site particle numbers (a)  $P(0)$ , (b)  $P(1)$ , and (c)  $P(2)$  vs  $T$  and  $U$  in the half-filled  $SU(4)$  Hubbard model. Due to the particle-hole symmetry,  $P(0) = P(4)$ , and  $P(1) = P(3)$ , and  $2P(0) + 2P(1) + P(2) = 1$ . The lattice size is  $L \times L$  with  $L = 10$ .

Figs. 5(a) and 5(b), respectively. Only the weak and intermediate interaction regimes with  $2 \leq U/t \leq 12$  are considered here. In the  $SU(4)$  case, when  $U/t < 6$ , the energy scale of  $\Delta_s$  is very small, and thus the peak location is beyond the temperature scope  $T/t > 0.1$  in our simulations. Compared to the  $SU(2)$  case,  $\Delta_s$  in the  $SU(4)$  case is significantly weakened. For example, the peak in the  $SU(2)$  Hubbard model is located around  $T_p/t \approx 0.3$  when  $U/t = 4$  as simulated in Ref. [43].

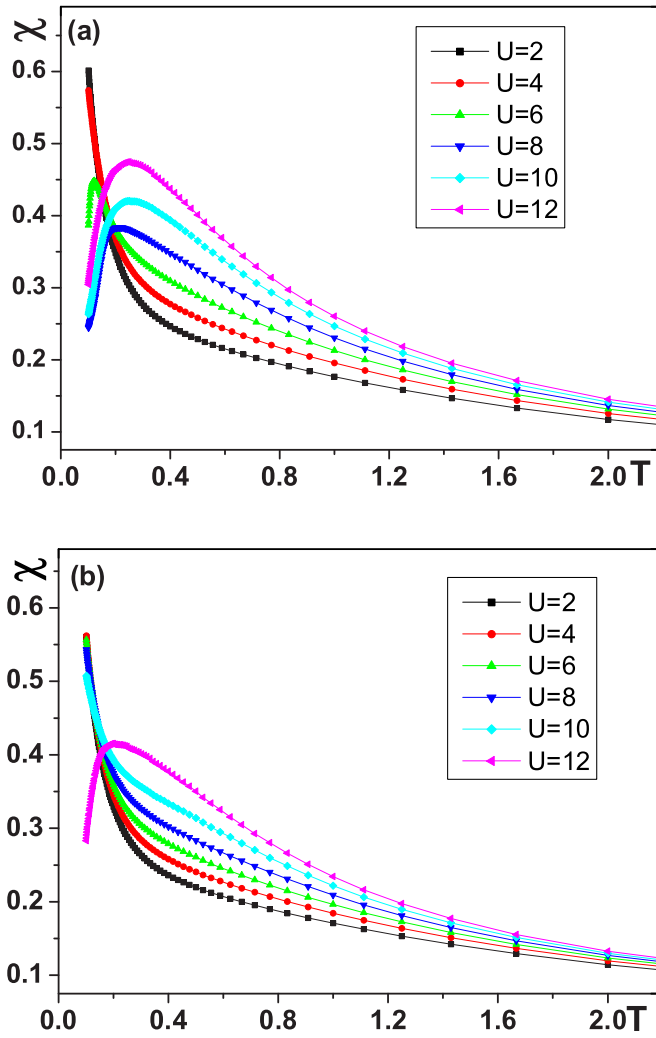


FIG. 5. (Color online) The uniform spin susceptibilities vs  $T$  for various  $U$  in the half-filled (a) SU(4) and (b) SU(6) Hubbard models. The system size is  $L \times L$  with  $L = 10$ . Error bars are smaller than the data points.

Nevertheless, the peak locations in the interaction regime  $6 < U/t < 12$  have already become visible at temperatures  $T_p/t > 0.1$ . Furthermore, the magnitude of  $T_p$  and the peak of  $\chi_{SU(4)}$  increases with  $U$ , which shows the enhancement of the AF correlations. In the SU(6) case, the AF correlations are further weakened compared to the SU(4) case: among the curves in Fig. 5(b), only the one with  $U/t = 12$  exhibits a peak visible at temperatures  $T_p/t > 0.1$ . This indicates the weakening of the spin energy scale  $\Delta_s$  in the intermediate interaction regime with increasing the number of fermion components.

### B. AF structure factors

We use the AF structure factor  $S_{SU(2N)}(\mathbf{Q})$  defined with staggered wave vector  $\mathbf{Q} = (\pi, \pi)$  to describe the AF correlations. In Fig. 6(a), the curves of the AF structure factor v.s.  $T$  are plotted at  $U/t = 12$  in both the SU(4) and SU(6) cases. Both  $S_{SU(4)}(\mathbf{Q})$  and  $S_{SU(6)}(\mathbf{Q})$  increase monotonically with the decrease of  $T$ , which indicates the development of AF correlations. At a fixed  $T$ ,  $S_{SU(4)}(\mathbf{Q})$  is stronger than  $S_{SU(6)}(\mathbf{Q})$ ,

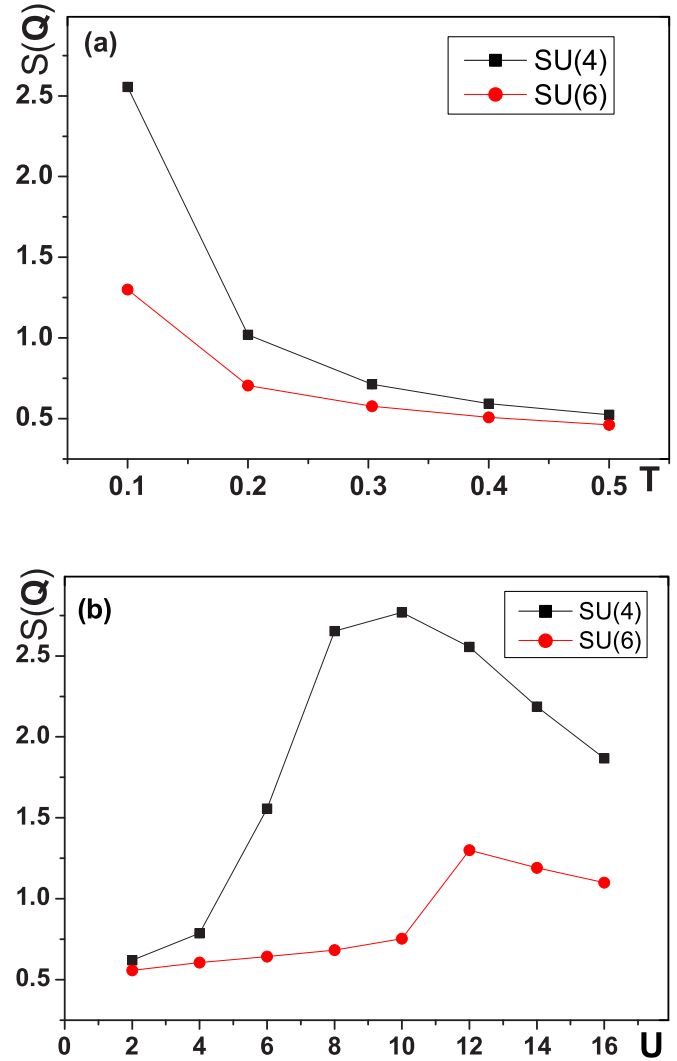


FIG. 6. (Color online) The AF structure factors  $S_{SU(2N)}(\mathbf{Q})$  with  $\mathbf{Q} = (\pi, \pi)$ : (a) as a function of  $T$  at fixed  $U/t = 12$ , and (b) as a function of  $U$  at fixed  $T/t = 0.1$  in the half-filled SU(4) and SU(6) Hubbard models. The system size is  $L \times L$  with  $L = 10$ . Error bars are smaller than the data points.

which becomes even more prominent at low temperatures. This is consistent with the picture that increasing the number of fermion components suppresses AF correlations.

In Fig. 6(b), the dependence of  $S_{SU(2N)}(\mathbf{Q})$  on  $U$  at a fixed temperature,  $T/t = 0.1$ , is plotted in both SU(4) and SU(6) cases, where the  $U$  dependencies exhibit a nonmonotonic behavior. At small  $U$ ,  $S_{SU(4)}(\mathbf{Q})$  and  $S_{SU(6)}(\mathbf{Q})$  increase with  $U$ . In this weak interacting regime,  $\Delta_c \simeq \Delta_s < T = 0.1t$ , and thus increasing  $U$  enhances the spin energy scale but suppresses density fluctuations, which facilitates to build up the AF correlation. Again, the enhancement of the AF correlation is more prominent in the SU(4) case than in the SU(6) case. An interesting feature is that the rates of increase jump at  $U/t \approx 4$  in the SU(4) case, and at  $U/t \approx 10$  in the SU(6) case. This may be due to a rapid increase of the density channel energy scale  $\Delta_c$ , which indicates the crossover from the weak interaction regime to the intermediate interaction regime. The AF in the weak interaction regime is due to Fermi surface nesting, and it evolves to the local moment physics as

$U$  enters the intermediate interaction regime. At large values of  $U$ ,  $\Delta_s \simeq J = 4t^2/U$  decreases with the increase of  $U$ . Thermal fluctuations are described by the parameter  $T/J$ , and thus increasing  $U$  effectively enhances thermal fluctuations.

On the other hand, the zero-temperature projector QMC results [55] show that the AF long-range orderings reach the maxima around  $U/t \approx 8$  and 10 in the SU(4) and SU(6) cases, respectively. The AF ordering is then suppressed by further increasing  $U$ , which is an effect of quantum fluctuations. In the SU(6) case, the AF long-range order is even completely suppressed around  $U/t \approx 15$  at zero temperature. This is because when deeply inside the Mott-insulating regime, the number of superexchange processes between two adjacent sites increases rapidly with the number of fermion components, which indicates the enhancement of quantum fluctuations. Combining both effects of quantum and thermal fluctuations, the AF correlations are weakened with increasing  $U$  in the strong interaction regime.

### VIII. DISCUSSIONS AND CONCLUSIONS

So far, we have only considered the homogeneous lattice system for the half-filled SU( $2N$ ) Hubbard models. In real optical lattices, there is also a harmonic confining potential  $V(\mathbf{r}) = \frac{1}{2}m\omega_\tau^2 r^2$ , which makes the system inhomogeneous and corresponds to a site-dependent chemical potential. If the density channel gap  $\Delta_c$  is large, a large region of the half-filled Mott-insulating state can exist in the central region of the trap and extends out. Due to the gap of  $\Delta_c$ , the compressibility of the Mott-insulating state vanishes at zero temperature and is exponentially suppressed as  $e^{-\frac{\Delta_c}{k_B T}}$  at  $T < \Delta_c$ , thus the filling number exhibits a plateau of  $N$  particles per site with a radius roughly  $r_M = \sqrt{\frac{2\Delta_c}{m\omega_\tau^2}}$ . Within this half-filled Mott-insulating region, the thermodynamic properties simulated above, such as the Pomeranchuk effect, still qualitatively apply. However, outside this Mott-insulating region, the particle number density is reduced from half filling, i.e., doping is introduced. In particular, near the edge of the system, the particle filling number drops to zero. As is well-known, the ground state and low-energy properties of doped Mott insulators are a major challenge to contemporary condensed matter physics. The particle-hole symmetry is also broken in the doped case, and thus the sign problem appears except in one dimension and QMC simulations are no long applicable at low temperatures. In the doped case, even though the Mott-insulating phase does not exist, strong interactions still enhance the tendency of localization of particles and then the spin channel mostly contributes to the entropy, and thus the Pomeranchuk effect should still survive. For example, in the one-dimensional case where the sign problem disappears even away from half filling, the QMC results still show the prominent feature of the Pomeranchuk effect in the SU( $2N$ ) Hubbard model [61].

In summary, we have performed a systematic DQMC simulation study of thermodynamic properties of the half-filled SU( $2N$ ) Hubbard model on a square lattice. Various thermodynamic behaviors including the entropy-temperature relation, the isoentropy curve, and the probability distribution of the on-site occupation number have been simulated, which demonstrate the Pomeranchuk effect is facilitated with

increasing fermion components. Based on the density and spin energy scales, we have analyzed the thermodynamic properties in weak and strong interaction regimes. In the weak interaction regime, the physics is characterized by the Fermi surface nesting, while in the strong interaction regime the physics is mostly in the local moment picture. Additionally, in our simulations the uniform spin susceptibilities and the AF structure factors both exhibit qualitatively different behaviors in weak and strong interaction regimes. Theoretical analysis as well as DQMC simulations show that the interaction strength separating weak and strong interaction regimes increases with the number of fermion components.

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### APPENDIX: AN EXACT HUBBARD-STRATONOVICH DECOMPOSITION FOR SU(4) AND SU(6) HUBBARD INTERACTIONS

For the SU(2) case, the HS transformation is usually performed by using the discrete Ising fields [47,48]. However, the decomposition in spin channel can not be easily generalized to the SU( $2N$ ) case due to the increase of spin components. Instead, we choose an discrete HS decomposition in the density channel at the price of involving complex numbers as used in Ref. [62]. The HS transformation for a half-filled SU( $2N$ ) Hubbard model reads:

$$e^{-\frac{\Delta\tau U}{2}(n_j - N)^2} = \frac{1}{4} \sum_{l=\pm 1, \pm 2} \gamma_j(l) e^{i\eta_j(l)(n_j - N)}, \quad (\text{A1})$$

where two sets of discrete HS fields  $\gamma$  and  $\eta$  are employed.

However, the HS decomposition with an error of order  $(\Delta\tau)^4$  in Ref. [62] is not exact. In Ref. [55], a new HS decomposition was proposed with a new set of parameters, which is exact for the SU(4) and SU(6) Hubbard interactions. The Ising fields are defined as follows

$$\begin{aligned} \gamma(\pm 1) &= \frac{-a(3 + a^2) + d}{d}; \\ \gamma(\pm 2) &= \frac{a(3 + a^2) + d}{d}; \\ \eta(\pm 1) &= \pm \cos^{-1} \left\{ \frac{a + 2a^3 + a^5 + (a^2 - 1)d}{4} \right\}; \\ \eta(\pm 2) &= \pm \cos^{-1} \left\{ \frac{a + 2a^3 + a^5 - (a^2 - 1)d}{4} \right\}, \end{aligned}$$

where  $a = e^{-\Delta\tau U/2}$ , and  $d = \sqrt{8 + a^2(3 + a^2)^2}$ .



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