Pomeranchuk Cooling of SU(2N) Ultracold Fermions in Optical Lattices

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(Received 8 April 2013; revised manuscript received 5 May 2013; published 29 May 2013)

We investigate the thermodynamic properties of a half-filled SU(2N) Hubbard model in the two-dimensional square lattice by the method of the determinant quantum Monte Carlo simulation, which is free of the fermion "sign problem." The large number of hyperfine-spin components enhances spin fluctuations, which facilitates the Pomeranchuk cooling to temperatures comparable to the superexchange energy scale in the case of SU(6). Various physical quantities including entropy, charge fluctuations, and spin correlations are calculated.

DOI: 10.1103/PhysRevLett.110.220401 PACS numbers: 03.75.Ss, 37.10.Jk, 71.10.Fd

The SU(2N) and Sp(2N) symmetries are usually studied in high energy physics. They were introduced to condensed matter physics originally as a mathematic convenience. For example, large-N analysis was performed for the SU(2N) symmetric Heisenberg models to systematically handle strong correlation effects [1–4], while realistic electron systems are usually only SU(2) invariant. However, with the recent development of the ultracold atom physics, fermion systems with SU(2N) and Sp(2N) symmetries are not just of purely academic interests but are currently under experimental investigations. It was first pointed out in Ref. [5] that large spin alkali and alkaline-earth fermion systems can exhibit these high symmetries. For example, a generic Sp(4) or isomorphically SO(5) symmetry is proved in fermion systems with the hyperfine-spin $F = 3/2$ without fine-tuning [5,6]. This Sp(4) symmetry can be further augmented to SU(4) for alkaline-earth fermions, such as ^{135}Ba, ^{137}Ba, and ^{201}Hg, because their interactions are hyperfine-spin independent [5]. Experimentally, both the fermionic atoms of ^{173}Yb and ^{87}Sr have been cooled down to quantum degeneracy [7–9]. The ^{173}Yb ($F = I = 5/2$) and ^{87}Sr ($F = I = 9/2$) systems exhibit the SU(6) and SU(10) symmetries, respectively. Using alkaline-earth fermions to study the SU(2N) symmetry was also proposed in Ref. [10].

The SU(2N) Hubbard model exhibits interesting phenomena that are absent in the standard SU(2) formulation. It is known that quantum spin fluctuations are enhanced by the large number of fermion components [11]. This effect gives rise to exotic quantum magnetism in large-spin ultracold fermi systems with high symmetries [12–19]. For example, various SU(2N) valence-bond solid and spin liquid states have been proposed that have not been observed in solid state systems before [15,20,21]. In addition, as we will show below, the multicomponent nature of the SU(2N) Hubbard model also significantly lowers the charge gap of the Mott-insulating states at the intermediate interaction strengths comparable to the bandwidth.

In this Letter, we focus on the temperature regime ($t > T \sim J$), which is of current experimental interest. Here, t denotes the hopping integral of the Hubbard model, $J = 4t^2/U$ is the antiferromagnetic exchange energy scale, and U is the on-site repulsion. The thermodynamic properties of the half-filled SU(2N) Hubbard model in the 2D square lattice are studied by determinant quantum Monte Carlo (DQMC) simulations [22,23], which is an unbiased, nonperturbative method. It is free of the sign problem at half-filling; thus, high numerical precision can be achieved down to low temperatures ($T/t \sim 0.1$). [Recently, the high temperature properties of the SU(2N) Hubbard model have been studied from series expansions, which are only accurate at $T \gg \max(t, U)$ [24].] Special attention is devoted to the interaction-induced adiabatic coolings. We find that the system can be cooled down to the temperature scale at J from an initial temperature accessible in current experiments. This Pomeranchuk cooling effect, although very weak in the SU(2) Hubbard model [25–27], is enhanced in the SU(6) case.

We consider the following SU(2N) Hubbard model defined in the 2D square lattice at half-filling 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 α runs over the $2N$ components, $\langle i, j \rangle$ denotes the summation over the nearest neighbors, and n_i is the total particle number operator on site i defined as

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$n_i = \sum_{\alpha=1}^{2N} c_{i\alpha}^\dagger c_{i\alpha}$. The chemical potential μ is set to 0 and thus does not appear explicitly. Equation (1) is invariant under the particle-hole transformation in bipartite lattices. Similarly to the case of SU(2), it is easy to prove that the sign problem is also absent for the half-filled SU($2N$) Hubbard model of Eq. (1) in bipartite lattices in the DQMC simulations.

Below, we will present our DQMC simulations of thermodynamic quantities of the SU($2N$) Hubbard model with $2N = 4$ and 6 on a $L \times L$ square lattice with the periodical boundary condition. The second order Suzuki-Trotter decomposition is used. The Trotter steps are taken to be $\Delta\tau = \beta/M$, where $\beta = 1/T$ is the inverse of the temperature T and M ranges from 30 to 150, depending on temperatures. We have checked that the simulation results converge with varying the values of $\Delta\tau$. Instead of using the Hubbard-Stratonovich transformation in the spin channel [28], we adopt the Hubbard-Stratonovich transformation in the charge channel, which maintains the SU($2N$) symmetry explicitly [29]. This method gives rise to errors on the order of $(\Delta\tau)^4$.

Before presenting numerical results, let us explain qualitatively how the SU($2N$) generalization of the Hubbard model makes their charge and magnetic properties different from those of the SU(2) case. When deeply inside the Mott-insulating state, magnetic properties at low temperatures are determined by superexchange processes. The number of superexchange processes between a pair of nearest-neighbor sites in the SU($2N$) case scales as N^2. This means that the SU($2N$) generalization enhances magnetic quantum fluctuations and thus weakens, or even completely suppresses, the long-range antiferromagnetic (AF) correlations. These strong magnetic fluctuations greatly enhance the entropy in the the temperature regime ($U > T > J$), which is high enough to suppress short-range AF correlations but not sufficient to unfreeze charge fluctuations.

The charge properties in the Mott-insulating state are characterized by the charge gap Δ_c: the energy cost to add a particle or a hole into the system. The half-filling case is a particle-hole symmetric point, and thus a particle or hole excitation each cost the same energy for the grand canonical Hamiltonian Eq. (1). In the atomic limit ($U/t \to \infty$), the charge gap is $\Delta_c \to U/2$, which is independent of $2N$. However, for the intermediate interactions comparable with the bandwidth, propagations of the extra particle (hole) in the AF background can significantly lower the charge gap. In Fig. 1(a), we compare the hopping of an extra hole in the AF background of the half-filled SU(2) and SU(4) Mott insulators. In the SU(4) case, there is more than one way for the hole to hop from one site to another. The mobility of the extra hole is increased, and thus, in the SU($2N$) Mott-insulating state, the charge gap is much lower compared to the SU(2) case. We perform the zero temperature projector QMC calculations to extract the charge gap from the unequal-time single-particle correlation functions (see the Supplemental Material [30]) as shown in Fig. 1(b), which verifies the above argument. Although the charge gap is a ground state property, it is closely related to the thermodynamic properties and Pomeranchuk cooling in the temperature regime we will study ($J < T < U$). Below, we will show that the differences of the magnetic and charge properties between the SU($2N$) and SU(2) cases facilitate the Pomeranchuk cooling.

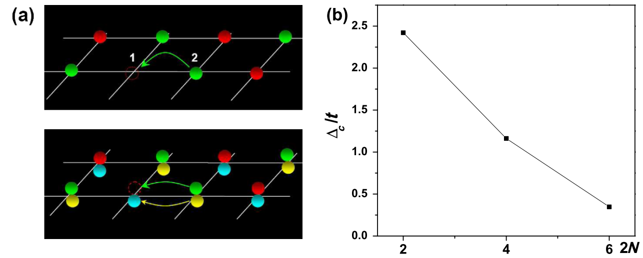

FIG. 1 (color online). (a) Sketches of a hole hopping in the SU(2) (up) and SU(4) (down) AF backgrounds, respectively. (b) Charge gaps as a function of $2N$ at $L = 10$ and $U/t = 8$.

Now, we address the possibility of cooling down the system by adiabatically increasing interactions. For spinful fermion systems (e.g., ^{3}He), the Pomeranchuk effect refers to the fact that increasing temperatures can lead to solidification because the entropy (per particle) in the localized solid phase is larger than that of the itinerant Fermi liquid phase. The reason is that, in the Fermi liquid phase, only fermions close to Fermi surfaces within T contribute to entropy. In solids however, each site contributes to nearly $\ln 2 \approx 0.69$ if T is comparable to the spin exchange energy scale of J, which is much smaller than the Fermi energy. In the lattice systems near or at half-filling, increasing interactions suppresses charge fluctuations and drives systems to the Mott-insulating state; thus, we would expect Pomeranchuk cooling while adiabatically increasing interactions [31,32]. However, the situations are complicated by the AF spin correlations, which lift the huge spin degeneracy and reduce the entropy in the Mott-insulating state. Actually, for the SU(2) Hubbard model, both at 2D and 3D, DQMC simulations show that the effect of Pomeranchuk cooling is not obvious with interactions up to $U/t \sim 10$ [25,26,33].

To investigate the different behaviors between the SU(2) and SU($2N$) (say, $2N = 6$) fermions during the Pomeranchuk cooling, we compare the "entropy capability" (average entropy per atoms) for the half-filled SU (2) and SU(6) Mott-insulating states at the same temperature T and U. We focus on the temperature regime ($J < T < U$). For a certain T, the entropy of the Mott-insulating state comes from two channels: the spin channel dominated by the spin degeneracy and the charge channel determined by excitations above the charge gap. As we analyzed above, the AF correlations, which lift the spin degeneracy in the SU(2) case, are weakened by the SU($2N$) symmetry. Thus, the entropy from the spin contribution in a half-filled SU(6) Mott insulator is larger than that of the SU(2) case. This indicates that the SU(6) Mott insulators have more "entropy capacity" than the SU(2) ones. For example, in the single-atom limit, the spin entropies per atom for SU(2) and SU(6) saturate to the values of $S_{\mathrm{SU}(2)} = \ln[C_2^1] = 0.693$ and $S_{\mathrm{SU}(6)} = \ln[C_6^3]/3 = 0.998$, respectively, for temperature $T \gg J$. Considering the charge channel will further strengthen this tendency. Since the charge gap of the SU(6) Mott-insulating state is smaller than that of the SU(2) case at the same value of U, it is easier to create excitations above the charge gap in the SU(6) case, which further increases entropy. The larger entropic capability of the SU(6) Mott-insulating state indicates that it is easier to exhibit the Pomeranchuk effect.

We have confirmed the above picture by performing DQMC simulations. The entropies of the SU(6) Hubbard model are calculated for various parameter values of T and U, and the isoentropy curves are displayed in Fig. 2. The simulated entropy per particle (not per site) is defined as $S_{\mathrm{SU}(2N)} = S/(NL^2)$, where S is the total entropy in the lattice. It is calculated from the formula

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

where ln4 is the entropy at the infinite temperature or, equivalently, $T \gg U$; $E(T)$ denotes the average internal energy per particle at temperature T. For low values of the entropy, adiabatically increasing U leads to a significant cooling to a temperature comparable to the magnetic superexchange scale J, which is an important goal in current cold atom experiments. This is of direct relevancy to the current experimental progress in ultracold ^{173}Yb atoms [7,34].

Next, we study particle number fluctuations for the half-filled SU($2N$) Hubbard model. The normalized on-site particle fluctuations are defined as

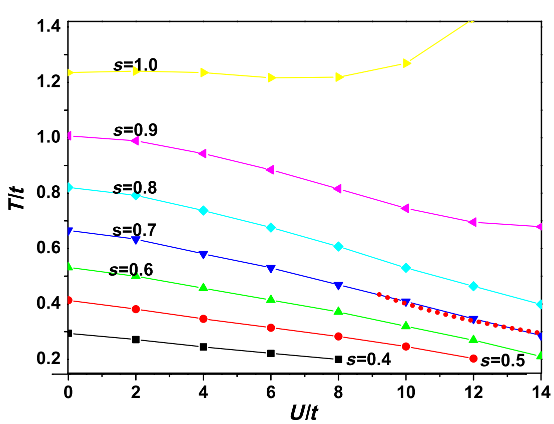

FIG. 2 (color online). The isoentropy curves for the half-filled SU(6) Hubbard model on a 10×10 square lattice. The dashed line denotes the spin superexchange scale in the strong coupling regime $J/t = 4t/U$.

$$\delta_{\mathrm{SU}(2N)} = \sqrt{\frac{\langle n_i^2 \rangle - \langle n_i \rangle^2}{N}}, \qquad (3)$$

where $\langle n_i \rangle = N$. At $T \to \infty$, $\delta_{\mathrm{SU}(2N)}$ can be calculated exactly. It is independent of $2N$ as $\delta_{\mathrm{SU}(2N)}(T \to \infty) = (\sqrt{2}/2) \approx 0.71$, which acts as an upper bound on the fluctuations. Similarly, at $U = 0$, $\delta_{\mathrm{SU}(2N)} = \sqrt{2}/2$ and is independent of both $2N$ and T. For the general case, we plot the DQMC simulation results of δ at a relatively weak interaction strength of $U/t = 4$ over a large range of temperatures seen in Fig. 3(a). For all the cases, $\delta_{\mathrm{SU}(2N)}$ is suppressed by U away from the upper limit of $\sqrt{2}/2$. For the cases of SU(4) and SU(6), $\delta_{\mathrm{SU}(2N)}(T)$ first falls as T increases, which is a reminiscence of the Pomeranchuk effect. Then, after reaching a minimum at T comparable to t, $\delta_{\mathrm{SU}(2N)}$ grows with increasing T. This indicates that fermions are localized most strongly at an intermediate temperature scale at which the spin channel contribution to entropy dominates. In comparison, the nonmonotonic behavior of $\delta_{\mathrm{SU}(2N)}$ is weak in the SU(2) case. The above data agree with the picture that large values of $2N$ enhance spin fluctuations and thus the Pomeranchuk effect. We also calculate the local particle number fluctuations in a small subvolume: $\delta_{\mathrm{sub}} = \sqrt{[\langle \hat{n}_{\mathrm{sub}}^2 \rangle - \langle \hat{n}_{\mathrm{sub}} \rangle^2]/\langle \hat{n}_{\mathrm{sub}} \rangle}$ ($\hat{n}_{\mathrm{sub}}$ is the total particle number operator within the subvolume).

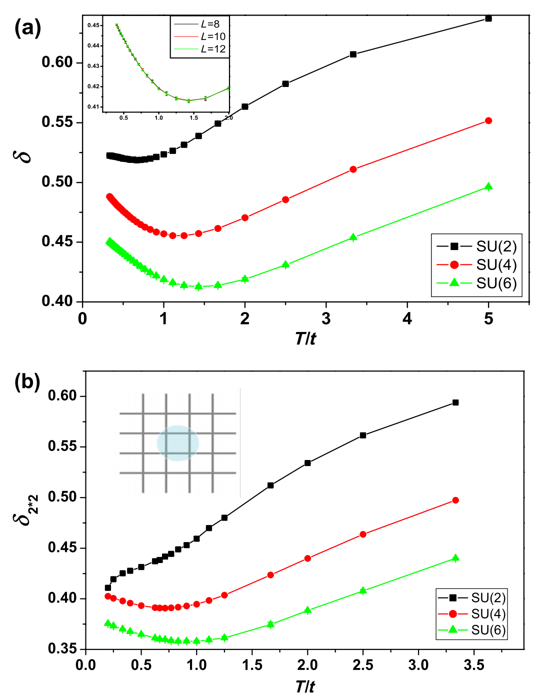

FIG. 3 (color online). Particle number fluctuations vs T with parameters $U/t = 4$ and different values of $2N$ on a 10×10 lattice. (a) The on-site density fluctuations $\delta_{\mathrm{SU}(2N)}(T)$. The inset shows the convergence of $\delta_{\mathrm{SU}(6)}(T)$ with $L = 8$, 10, and 12 for the SU(6) case. (b) The local particle number fluctuations in a 2×2 subvolume.

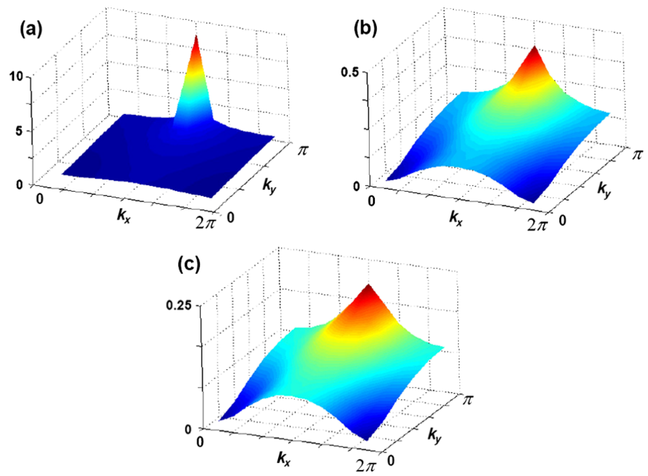

FIG. 4 (color online). The normalized spin structure factor $S(\vec{q})$ for the half-filled SU($2N$) Hubbard models with $2N$ equal to (a) 2, (b) 4, and (c) 6. Parameter values are $T/t = 0.1$ and $U/t = 8$.

As shown in Fig. 3(b), for the SU(4) and SU(6) cases, the local density fluctuations in a 2×2 sublattice $\delta_{2\times2}$ also exhibit nonmonotonic behavior similarly to the case of the on-site density fluctuation.

Next, we study spin correlations of the SU($2N$) Hubbard model. The SU($2N$) generators can be represented through fermion operators $c_{i,\alpha}(\alpha = 1 \sim 2N)$ as $S_{\alpha\beta,i} = c^\dagger_{\alpha,i}c_{\beta,i} - (1/2N)\delta_{\alpha\beta}n_i$. There are only $(2N)^2 - 1$ independent operators due to the constraint $\sum_\alpha S_{\alpha\alpha} = 0$. They satisfy the commutation relations $[S_{\alpha\beta,i}, S_{\gamma\delta,j}] = \delta_{i,j}(S_{\alpha\delta,i}\delta_{\gamma\beta} - S_{\gamma\beta,i}\delta_{\alpha\delta})$. We define the SU($2N$) version of the two-point equal-time spin-spin correlation as

$$S_{\rm spin}(i,j) = \frac{1}{(2N)^2 - 1}\sum_{\alpha,\beta}\langle S_{\alpha\beta,i}S_{\beta\alpha,j}\rangle. \quad (4)$$

The spin structure factors $S_{{\rm SU}(2N)}(\vec{q})$ are calculated at half-filling and a low temperature, which are defined as

$$S_{{\rm SU}(2N)}(\vec{q}) = \frac{1}{NL^2}\sum_{\vec{i},\vec{j}} e^{i\vec{q}\cdot\vec{r}} M_{\rm spin}(i,j), \quad (5)$$

where $\vec{r}$ is the relative vector between sites i and j. The distributions of $S_{{\rm SU}(2N)}(\vec{q})$ with $2N = 2, 4, 6$ are plotted in Figs. 4(a)–4(c), respectively. The sharpness of the peaks at $\mathbf{q} = (\pi, \pi)$ indicates the dominant AF correlations in all the cases. With increasing $2N$, peaks are broadened, showing a weakening of the AF correlations.

The current experimental limit to the entropy per particle for the two-component systems is $S_{{\rm SU}(2)} \sim 0.77k_B$. The corresponding temperature scale is $T \sim t$, which is still larger than J [35]. In contrast, as we analyzed above, the SU(6) Mott-insulating state has more entropy capacity, which means that, for a fixed entropy per atom, the corresponding temperature of the half-filled SU(6) Mott-insulating state is lower than that of the SU(2) case. As shown in Fig. 2, for $S_{{\rm SU}(6)} \sim 0.77k_B$, the corresponding temperature of the Mott-insulating state ($U/t = 12$) can reach the border of the magnetic superexchange scale J. As for the experimental consequences of the Pomeranchuk cooling, although it is difficult to directly measure temperatures in the lattice, the nonmonotonic behavior of the local particle fluctuations, shown in Figs. 3(a) and 3(b), can be tested by high-resolution *in situ* measurements which have been used to observe the antibunching in ultracold atom Fermi gases [36]. Repeated measurements of the local particle numbers of identically prepared systems give rise to particle fluctuations within the observed volume, which may contain one or several lattice sites. Recently, the Pomeranchuk cooling has been observed in ^{173}Yb fermions in optical lattice [SU(6) Hubbard model]. However, we should point out an important difference between the experiment and our calculation, namely, that the filling factor in the experiment [34] is $1/6$ (one fermion per site) as opposed to the assumed half-filling in our simulations.

In conclusion, we have performed DQMC simulation for the thermodynamic properties of the 2D SU($2N$) Hubbard model at half-filling in the temperature regime of direct interest to current experiments. The large numbers of fermion components enhance spin fluctuations, which facilitates the Pomeranchuk cooling to temperatures comparable to the superexchange energy scale. We have focused on half-filling, although it is interesting to ask whether the Pomeranchuk cooling can appear in other filling factors, especially in the the case of $1/6$ filling corresponding to one atom per site in the SU(6) model. In this case, DQMC calculation is plagued by the sign problem. Nevertheless, in some situations, for example, at high temperatures or small values of U, DQMC calculation can still give rise to reliable results if the sign problem is not severe.

We acknowledge J. Hirsch, D. Greif, R. Scalettar, and Y. Takahashi for helpful discussions. C. W. thanks S. Kravec for improving the language of this Letter. This work was supported by the NSF Grant No. DMR-1105945 and the AFOSR Contract No. FA9550-11-1-0067 (YIP) Program. Z. C. is also supported by the German Research Foundation through DFG FOR 801.

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[1] D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).
[2] I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988).
[3] N. Read and S. Sachdev, Nucl. Phys. **B316**, 609 (1989).
[4] N. Read and S. Sachdev, Phys. Rev. Lett. **66**, 1773 (1991).
[5] C. Wu, J. P. Hu, and S. C. Zhang, Phys. Rev. Lett. **91**, 186402 (2003).
[6] C. Wu, Mod. Phys. Lett. B **20**, 1707 (2006).

[7] S. Taie, Y. Takasu, S. Sugawa, R. Yamazaki, T. Tsujimoto, R. Murakami, and Y. Takahashi, Phys. Rev. Lett. **105**, 190401 (2010).
[8] B. J. DeSalvo, M. Yan, P. G. Mickelson, Y. N. Martinez de Escobar, and T. C. Killian, Phys. Rev. Lett. **105**, 030402 (2010).
[9] H. Hara, Y. Takasu, Y. Yamaoka, J. M. Doyle, and Y. Takahashi, Phys. Rev. Lett. **106**, 205304 (2011).
[10] 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).
[11] C. Wu, Nat. Phys. **8**, 784 (2012).
[12] C. Wu, Phys. Rev. Lett. **95**, 266404 (2005).
[13] M. A. Cazalilla, A. F. Ho, and M. Ueda, New J. Phys. **11**, 103033 (2009).
[14] S. R. Manmana, K. R. A. Hazzard, G. Chen, A. E. Feiguin, and A. M. Rey, Phys. Rev. A **84**, 043601 (2011).
[15] H.-H. Hung, Y. Wang, and C. Wu, Phys. Rev. B **84**, 054406 (2011).
[16] G. Szirmai, E. Szirmai, A. Zamora, and M. Lewenstein, Phys. Rev. A **84**, 011611 (2011).
[17] E. Szirmai and M. Lewenstein, Europhys. Lett. **93**, 66005 (2011).
[18] M. Colome-Tatche, C. Klempt, L. Santos, and T. Vekua, New J. Phys. **13**, 113021 (2011).
[19] F. F. Assaad, Phys. Rev. B **71**, 075103 (2005).
[20] S. Chen, C. Wu, S. C. Zhang, and Y. Wang, Phys. Rev. B **72**, 214428 (2005).
[21] M. Hermele and V. Gurarie, Phys. Rev. B **84**, 174441 (2011).
[22] D. J. Scalapino, arXiv:cond-mat/0610710.
[23] J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).
[24] K. R. A. Hazzard, V. Gurarie, M. Hermele, and A. M. Rey, Phys. Rev. A **85**, 041604 (2012).
[25] A.-M. Daré, L. Raymond, G. Albinet, and A.-M. S. Tremblay, Phys. Rev. B **76**, 064402 (2007).
[26] T. Paiva, R. Scalettar, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **104**, 066406 (2010).
[27] E. Khatami and M. Rigol, Phys. Rev. A **84**, 053611 (2011).
[28] J. E. Hirsch, Phys. Rev. B **28**, 4059 (1983).
[29] F. F. Assaad, arXiv:cond-mat/9806307.
[30] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.110.220401 for the derivation of the charge gap.
[31] F. Werner, O. Parcollet, A. Georges, and S. R. Hassan, Phys. Rev. Lett. **95**, 056401 (2005).
[32] Y. Li, M. R. Bakhtiari, L. He, and W. Hofstetter, Phys. Rev. A **85**, 023624 (2012).
[33] T. Paiva, Y. L. Loh, M. Randeria, R. T. Scalettar, and N. Trivedi, Phys. Rev. Lett. **107**, 086401 (2011).
[34] S. Taie, R. Yamazaki, S. Sugawa, and Y. Takahashi, Nat. Phys. **8**, 825 (2012).
[35] R. Jördens *et al.*, Phys. Rev. Lett. **104**, 180401 (2010).
[36] T. Müller, B. Zimmermann, J. Meineke, J.-P. Brantut, T. Esslinger, and H. Moritz, Phys. Rev. Lett. **105**, 040401 (2010).