Artificial $SU(3)$ Spin-Orbit Coupling and Exotic Mott Insulators

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(Dated: September 18, 2018)

Motivated by recent progress in the realization of artificial gauge fields and $SU(N)$ Mott insulators using alkaline-earth-like atoms in optical lattices, we study the effect of spin-orbit coupling and onsite Hubbard interaction $U$ on $SU(3)$ fermionic systems using an unbiased real-space dynamical mean-field theory (DMFT) approach. We investigate the behavior of the local magnetization, double occupancies, and the triple occupancy versus the Hubbard interaction across the metal to Mott insulator transition. We map out the magnetic phase diagram in the large-$U$ limit and show that the spin-orbit coupling can stabilize long-range orders such as ferromagnet, spiral, and stripes with different orientations in $SU(3)$ Mott insulators.

PACS numbers: 71.30.+h, 71.10.Fd, 37.10.Jk

I. INTRODUCTION

Since the experimental observation of Bose-Einstein condensation\(^1\), ultracold atoms have attracted a lot of attention as a flexible playground to mimic various models of condensed matter physics\(^2\) and beyond\(^3\). The Haldane model is a fundamental model in the field of topological insulators which describes the transition between topologically distinct phases in the absence of net magnetic flux through the unit cell\(^4\). Thanks to the lattice-shaking technique and Floquet theory, the Haldane model which was initially considered difficult to realize is implemented in optical lattices and its phase diagram has been mapped out\(^5\). In the same spirit, although technically differently, the time-reversal-invariant Hofstadter Hamiltonian has been realized\(^6\text{-}^8\), the Chern number of the lowest Hofstadter band has been determined\(^9\), and the Berry curvature of the Bloch bands measured\(^10\). Going beyond Abelian gauge fields\(^11\), non-Abelian gauge fields for $SU(2)$ systems can also be engineered in optical lattices\(^12\text{-}^14\) leading, for example, to the prediction of the Hofstadter moth\(^12\).

The perfect decoupling of nuclear spin from electronic angular momentum in alkaline-earth atoms provides a unique possibility to study $SU(N)$ Mott insulators in optical lattices with $N$ as large as 10\textsuperscript{15}–17. Depending on the value of $N$ and the lattice geometry, phases such as multi-flavor magnetism\(^18\text{-}19\), valence-bond solid states\(^20\text{-}22\), and quantum spin liquids\(^23\text{-}26\) are predicted to emerge. While the strong spin-orbit coupling in $SU(2)$ Mott insulators leads to phases such as collinear, spiral, and tetrahedral spin orders\(^23\text{-}26\), in high-spin systems the phase diagram is expected to be richer not only in magnetic order but also with respect to topology. For instance, a translationally constant gauge field in an $SU(3)$ system can lead to non-trivial topological bands, in contrast to the $SU(2)$ case\(^27\). Proposals to realize effective $SU(3)$ spin-orbit coupling in optical lattices already exist\(^28\text{-}30\).

In this paper, we explore the $SU(3)$ Hubbard model on the triangular lattice at 1/3-filling subject to homogenous non-Abelian gauge fields, using the real-space dynamical mean-field theory (DMFT) approximation\(^31\text{-}32\). The method is applied to various 2-component models with spin-orbit coupling\(^25\text{-}33\text{-}34\). We have employed the exact diagonalization (ED) approach as the impurity solver. Although the $SU(3)$ Hubbard model without gauge fields has been investigated near 1/2-filling with anisotropic interactions\(^35\text{-}37\) and at 1/3-filling in the large-$U$ limit\(^18\text{-}19\text{-}38\), there are no results available across the metal to Mott insulator transition in the $SU(3)$-symmetric version. First, we set the gauge field to zero and show that the $SU(3)$ Hubbard model on the triangular lattice at 1/3-filling shows a transition from a metallic phase to Mott insulator with 3-sublattice magnetic order at the Hubbard interaction $U \sim 1.6t\text{.}$ We study the behavior of different local quantities such as the magnetization, double occupancies, and the triple occupancy versus $U$. Next, we analyze the effect of gauge fields on the emergence of exotic $SU(3)$ magnetism in the Mott regime. We find $SU(3)$ Mott insulators with long-range orders such as ferromagnetic, spiral, and stripes with different kinds of orientations.

II. HAMILTONIAN

We consider the Hamiltonian

$$H = -t \sum_{\langle r, r+\delta \rangle} \left( \Psi_r^\dagger \hat{T}_d \Psi_r + \text{H.c.} \right) + \frac{U}{2} \sum_r \Psi_r^\dagger \Psi_r \Psi_r^\dagger \Psi_r - \mu \sum_r \Psi_r^\dagger \Psi_r ,$$

(1)

where we have defined the $SU(3)$ creation field operator $\Psi_r = (c_{r, +1}, c_{r, 0}, c_{r, -1})$. The operators $c_{r, \alpha}^\dagger$ and $c_{r, \alpha}$ represent the fermionic creation and annihilation operators at the position $r$ with the flavor $\alpha = \pm 1, 0$. We define also the occupation operator $n_{r, \alpha} = c_{r, \alpha}^\dagger c_{r, \alpha}$. The position vector $r$ runs over the triangular lattice and the nearest-neighbor (NN) vector can have the values $\delta = \hat{x}, \hat{y}, \hat{x} + \hat{y}$ where $\hat{x}$ and $\hat{y}$ are the unit vectors according to the reference frame specified in Fig. 1 with the lattice constant set
but also interesting spin orders in where Fermi-liquid, superfluid, and the last term enables us to reach the desired filling by adjusting the chemical potential $\mu = U$ to a density of one fermion per lattice site. At the spin-orbit coupling $\kappa = 0$, one has $T_\gamma = \mathbb{1}$ and $T_x = T_x + y$, and hence the Hamiltonian is invariant under reflection with respect to the axis $(2x + y)$, i.e., the horizontal dashed line in Fig. 1. In addition, the Hamiltonian is invariant under reflection with respect to the $y$ axis, provided that we apply the transformation $\gamma \rightarrow -\gamma$ which maps $T_x \rightarrow T_y$. This allows one to limit $0 \leq \gamma < 0.5$ at $\kappa = 0$. The time-reversal operator is $\Theta = e^{-i\pi J_y K}$ where $J_y$ is the $y$-component of the spin operator and $K$ is the complex conjugate operator and we set $h = 1$. Under the time-reversal transformation the $SU(3)$ creation field operators transform as

$$\Theta \Psi^\dagger \Theta^{-1} = \left( c^\dagger_{\gamma r, -1}, -c^\dagger_{\gamma r, 0}, c^\dagger_{\gamma r, +1} \right) =: \Psi^\dagger (1 - 2J^2_y)$$

$$=: \Psi^\dagger \hat{\Theta} K$$

where $J_y$ and $\hat{\Theta}$ are the matrix representations of the operators $J_y$ and $\Theta$. Since the Gell-Mann matrices $\lambda_5$ is even under time-reversal, i.e., $\Theta \lambda_5 \Theta^{-1} = +\lambda_5$, the Hamiltonian (1) is not time-reversal-invariant for any finite $\gamma$ and $\kappa$.

III. METAL-INSULATOR TRANSITION

The $SU(3)$ Hubbard model at and near 1/2-filling with anisotropic interactions has already been studied in detail in Refs. 35-37 where Fermi-liquid, superfluid, paired Mott insulator, and color-selective Mott insulator phases are characterized. At 1/3-filling and in the large-$U$ limit, the fermionic $SU(3)$ Hubbard model can be effectively described by the $SU(3)$ Heisenberg model, which is shown to have 3-sublattice magnetic order on both square and triangular lattices18,38. Thermal fluctuations destabilize this 3-sublattice order into 2-sublattice order and subsequently into a paramagnetic phase19,42.

Nevertheless, the interaction-driven transition between the metal and the 3-sublattice order Mott insulator phase at 1/3-filling has not been addressed yet. In this section, we set the spin-orbit coupling $\gamma = \kappa = 0$ which
reduces the Hamiltonian (1) to the fermionic $SU(3)$ Hubbard model on the triangular lattice. We fix the inverse temperature to $\beta t = 20$. The ED impurity solver is used with 4 bath sites and the results are checked versus 5 bath sites. We consider $30 \times 30$ lattices with periodic boundary conditions. The results remain unchanged upon increasing the system size to $51 \times 51$.

We identify a phase transition from a metallic to a Mott insulator phase at $U_c \simeq 10.7t$ upon increasing the Hubbard interaction. The Mott insulator phase is characterized by the 3-sublattice order shown in Fig. 2a. The system consists of horizontal stripes with a sequence of, e.g., $A$, $B$, and $C$ stripes. We call this phase horizontal-stripe phase to be distinguished from more elaborate lattice patterns that we find in the next section. To reveal the pseudospin order we calculate the 8-dimensional pseudospin vector

$$S_\alpha := \frac{1}{2} \langle \Psi | \lambda \Psi \rangle$$

(4)

where $\lambda := (\lambda_1, \lambda_2, \ldots, \lambda_8)$ is a vector made of Gell-Mann matrices. The angle between pseudospin vectors is computed using the scalar product. The Mott insulator phase shows an in-plane 120° pseudospin order sketched in Fig. 2b. This is similar to the spiral long-range order in the $SU(2)$ Hubbard model on the triangular lattice. Due to the spontaneous breaking of the $SU(3)$ symmetry, the plane in which the pseudospin vectors lie is not unique. With our unbiased real-space DMFT method we have been able to generate different of these degenerate states. The trivial solution is the one where $\langle c_{r \alpha}^\dagger c_{r \beta} \rangle = 0$ for any $\alpha \neq \beta$ and consequently the pseudospin vectors lie in the $S_3-S_8$ plane, where $S_i$ stands for the unit vector in the $i$th direction in the pseudospin space. In this state, at each sublattice one of the flavors has the dominant density and the densities of the other two flavors are equal. Similar spiral orders for frustrated classical spin systems are recently created and detected in optical lattices.

There are three different double occupancies $D_1$, $D_2$, and $D_3$ corresponding to different $\alpha$ and $\beta$ in $\langle n_{r \alpha} n_{r \beta} \rangle$. In Fig. 2c, we have plotted the double occupancies, the triple occupancy $T := \langle n_{r+1 \alpha} n_{r,0} n_{r \beta} \rangle$ as well as the local magnetization $M := \langle S^\alpha \rangle$ versus the Hubbard interaction $U$. The three double occupancies are equal in the metallic phase and decrease upon increasing $U$ up to the transition point $U_c$. In the Mott phase, two of the double occupancies are equal and larger than the third one. Right above $U_c$, two of the double occupancies increase and the third one decreases sharply. At large values of $U$, the larger double occupancies decrease as power-law and the third one is negligible. The triple occupancy decreases exponentially versus $U$ and in the entire metallic phase can be fitted almost perfectly with the function $\langle n_{r \alpha} \rangle^3 e^{-0.3U/\gamma}$. The local magnetization $M$, similar to the double occupancies, changes sharply across the transition point and in the large-$U$ limit approaches the fully polarized value $1/\sqrt{3} \simeq 0.58$. We believe the data support a second order or very weakly first order transition.

IV. SPIN-ORBIT-COUPLED MOTT INSULATORS

We fix the Hubbard interaction to $U = 15t$ and explore the effect of the spin-orbit coupling on the 3-sublattice magnetic order with horizontal stripes discussed in the previous section. The inverse temperature is fixed to $\beta t = 20$. We have considered the ED impurity solver with 3 bath sites and checked the results versus 4 bath sites. We have mainly considered $30 \times 30$ lattices, periodic boundary conditions, and unit cells as large as $6 \times 3$. But we have checked for some selected points that the results remain unchanged upon increasing the system size to $48 \times 48$ and increasing the unit cell to $12 \times 6$. This allows us to find commensurate magnetic orders with relatively large periodicity.

In contrast to the $SU(2)$ systems where spins are 3-dimensional objects, the 8-dimensional nature of the pseudospin vectors in the $SU(3)$ systems make it difficult to identify and name the pseudospin order. We have mostly concentrated on the stabilization of different lattice patterns induced by the spin-orbit coupling. The pseudospin order is discussed only in some cases. For any values of $\gamma$ and $\kappa$, we always find that the norm of...
the pseudospin vector is the same on every lattice site.

We first set $\kappa = 0$ and study the effect of $\gamma$. In Fig. 3, we have plotted the ground state energy per lattice site $\epsilon$ shifted by $U/2$ versus $\gamma$, panel (a), as well as the schematic representation of different lattice patterns which appear, panels (b)-(d). We always find the pseudospin vector in the five dimensional $S_1 - S_3 - S_4 - S_6 - S_8$ space, i.e., $\langle S_2 \rangle = \langle S_3 \rangle = \langle S_4 \rangle = 0$. However, we do not exclude the possibility that there might be other degenerate solutions as the $SU(3)$ symmetry is not fully broken by $\gamma \neq 0$. Moreover, we find that the pseudospin vectors in the $\hat{y}$ direction always form an in-plane 120° order as depicted in Fig. 2b.

We discuss the simpler phases in Fig. 3a first. One can see from Fig. 3a that the ground state energy of the phase with horizontal stripes increases upon increasing $\gamma$. This phase is stable up to $\gamma \approx 1/12$ where a first order transition takes place. For $1/4 \lesssim \gamma \leq 5/12$, the system has a ferromagnetic order along the $\hat{x}$ direction and an in-plane 120° spiral order along the $\hat{y}$ direction. This phase is schematically displayed in Fig. 3b. The lattice comprises diagonal stripes with a sequence of a 3-color cycle. Due to the spontaneous breaking of the horizontal reflection symmetry, this state is degenerate with the one in which diagonal stripes are oriented along $\hat{x} + \hat{y}$ direction. We have explicitly checked this degeneracy. As the hopping matrices at $\gamma = 1/3$ and $\kappa = 0$ simplify to

$$\hat{T}_x = \hat{T}_{\hat{x} + \hat{y}} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \hat{T}_y = \hat{1}$$  \hspace{1cm} (5)$$
a diagonal-stripe phase in the vicinity of $\gamma = 1/3$ is what one would expect from a second order perturbation theory in the large-$U$ limit. The $SU(2)$ counterpart of such a phase would have the ferromagnetic and the antiferromagnetic orders along $\hat{x}$ and $\hat{y}$ directions and is found, for example, as a result of a Rashba-like spin-orbit coupling in both bosonic and fermionic systems. It is usually called collinear or nematic order.

For $5/12 \lesssim \gamma \lesssim 1/2$, we identify a phase with 6-sublattice order shown schematically in Fig. 3c. In contrast to the 3-sublattice order sketched in Fig. 2a, this is a phase with the length of the unit cell along $\hat{x}$ direction doubled. One can understand this phase as two penetrating rectangular lattices specified by black dotted lines and by orange dashed lines in Fig. 3c. On each rectangular lattice there is a ferromagnetic order along the horizontal direction and an in-plane 120° spiral order along the vertical direction, i.e., the pseudospin vectors at the sites $A$, $B$, and $C$ obey the relation $\hat{S}_A + \hat{S}_B + \hat{S}_C = 0$ and likewise for the pseudospin vectors at the sites $D$, $E$, and $F$. One notices that the norm of the pseudospin vector is the same on every lattice site. Each rectangular lattice represents horizontal stripes with a sequence of a 3-color cycle. Although the states over the two rectangular lattices are obviously coupled, we have not been able to find a specific relation between the pseudospin order at the sites $A$, $B$, and $C$ and the pseudospin order at the sites $D$, $E$, and $F$. One can interpret this state also over the full triangular lattice as consisted of horizontal stripes with a succession of a 6-color cycle. We refer to this state as nested horizontal stripes.

We proceed with the state which appears for $1/12 \leq \gamma \leq 1/4$ in Fig. 3a. The symmetry in this phase is quite reduced and the system shows an 18-sublattice order. This phase is schematically shown in Fig. 3d with a 6-site periodicity along $\hat{x}$ and a 3-site periodicity along $\hat{y}$ direction. To have a simpler understanding of this state, we have interpreted the triangular lattice again as two penetrating rectangular lattices specified by black dotted lines.
V. SUMMARY AND OUTLOOK

In recent years, there has been a noticeable development on realization of artificial gauge fields in optical lattices, which led to the implementation of the fundamental models such as the Haldane and Hofstadter Hamiltonians. Beside experimental achievements, there has been a number of experimental proposals and theoretical predictions especially for non-Abelian gauge fields and effective spin-orbit coupling in SU(2) and SU(3) systems. While the spin-orbit coupling in non-interacting systems is essential to realize topological bands, in strongly interacting regimes it can stabilize Mott insulators with exotic long-range orders.

In this work, we have investigated the fermionic SU(3) Hubbard model in the presence of spin-orbit coupling on the triangular lattice. The SU(3) Hubbard model shows a transition from a metallic phase to a Mott insulator, interestingly very close, which illustrates how different long-range orders become favorable in different spin-orbit coupling regimes.

We turn now to the case of finite $\kappa$. The Hamiltonian is invariant under the transformation $\kappa \rightarrow \kappa + 2$. In addition, we find that the phase diagram is symmetric with respect to $\kappa = 0$. Hence, we restrict $0 \leq \kappa \leq 1$. Upon introducing a finite value of $\kappa$, all the 8 components of the pseudospin vector become finite, making the recognition and the discussion of the pseudospin order more complicated. In the following we focus only on ordering patterns in real space.

We consider the values $\gamma = 0$, 1/6, 1/3, and 1/2 and study the effect of $\kappa$ on the different lattice patterns that we discussed. We find that the horizontal-stripe pattern in Fig. 2a as well as the diagonal-stripe pattern in Fig. 3b remain stable upon introducing the spin-orbit coupling $\kappa$. The phase diagram versus $\kappa$ at $\gamma = 1/2$ is presented in Fig. 4a. At $\gamma = 1/2$, an intermediate ferromagnetic phase appears for $0.62 \lesssim \kappa \lesssim 0.80$. Below and above this region we find the nested horizontal-stripe pattern sketched in Fig. 3c. The phase diagram versus $\kappa$ at $\gamma = 1/6$ is plotted in Fig. 4b. In the 12-sublattice order, see Fig. 3d, near $\kappa = 0$ and $\kappa = 1$, we detect a diagonal-stripe order and a nested diagonal-stripe order. In both phases, stripes are oriented in the $\hat{x} + \hat{y}$ direction and they are depicted in Figs. 4c and 4d.

In the nested diagonal-stripe state, the triangular lattice is seen as two penetrating rectangular lattices, each one forming a $(\hat{x} + \hat{y})$-oriented diagonal-stripe order. The phase diagram in Fig. 4b is approximately symmetric with respect to $\kappa = 1/2$, but this does not apply to physical quantities such as, for example, the ground state energy. Upon increasing $\kappa$ from 0 to 1/2 at $\gamma = 1/6$ the symmetry of the lattice is restored; first from the 12-sublattice order to the 6-sublattice order with nested diagonal stripes and subsequently to the 3-sublattice order with diagonal stripes.
which we have studied in details. The Mott phase has in-plane 120° spiral pseudospin order. The spin-orbit coupling drives this 3-sublattice Mott insulator to Mott states with various types of lattice patterns such as horizontal stripes and diagonal stripes with different orientations. In addition, we find more complex lattice orders which we have interpreted as two nested rectangular lattices with horizontal and diagonal stripes each. Due to the complex 8-dimensional nature of the pseudospin vector, the pseudospin order is discussed only in some cases where ferromagnetic, spiral, and cone orders are recognized. While this work is mainly devoted to the spin-orbit-coupled Mott insulators, we have shown that the Hamiltonian considered here has interesting topological features through the connection with the $SU(3)$ Hatsugai-Harper-Hofstadter-Hubbard model. The real-space DMFT method equipped with the continuous-time quantum-Monte-Carlo impurity solver can enable us to address edge states of interacting topological phases on cylindrical geometries. An alternative approach to discuss topological phase transitions would be the calculation of the Chern number, which is already formulated for $SU(3)$ systems in the non-interacting case\cite{17}. This could be extended to interacting phases using, for example, the effective topological Hamiltonian approach\cite{18}. It is left for future research to explore the topological properties of the model at finite spin-orbit coupling and different interaction strengths.

\section*{ACKNOWLEDGMENT}

We would like to thank Nathan Goldman, Bernhard Irsigler, Jaromir Panas, Christof Weitenberg, and Jun-Hui Zheng for useful discussions. This work was supported by the Deutsche Forschungsgemeinschaft via DFG FOR 2414 and the high performance computing center LOEWE-CSC.

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