Competing Charge and Magnetic Order in Fermionic Multi-Component Systems

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We consider the fermionic SU(3) Hubbard model on the triangular lattice in the presence of a three-sublattice staggered potential which provides the possibility to investigate the competition of charge and magnetic order in three-component systems. We show that depending on the strength of the staggered potential $\Delta$, the Hubbard interaction $U$ destablizes the band insulator (BI) at small $U$ into the Mott insulator (MI) at large $U$ in three different ways with different intermediate phases. This leads to a rich phase diagram in the $U$-$\Delta$ plane. Our results indicate that multi-component systems show not only exotic states in the Mott regime as has been considered previously, but also interesting competition between charge and magnetic orders.

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

The observation of Bose-Einstein condensation \cite{1} triggered a huge research interest in ultracold atoms trapped in optical lattices as flexible and highly controllable quantum simulators not only to mimic models of solid state physics but also to study systems which have no obvious solid state counterparts \cite{2-4}. Alkali and alkaline-earth-like atoms have up to $N=10$ internal states available, which due to the perfect decoupling of the nuclear spin from the electronic angular momentum can be used to simulate multi-component systems with an unprecedented SU($N$) symmetry \cite{5-7}. Theoretical predictions depending on the value of $N$ suggest multi-component magnetism \cite{8-12}, valence-bond solid states \cite{12-14}, and quantum liquids \cite{14-16} in the Mott regime. A three-component Fermi gas with SU(3) symmetry has been realized using $^6$Li atoms in high magnetic field \cite{17,18} and the fermionic SU(6) Hubbard model has been realized using $^{173}$Yb \cite{19}. In this work we demonstrate that multi-component systems show not only exotic phases in the Mott regime as has been discussed previously, but also interesting competition between charge and magnetic order with a possible emergence of charge-ordered magnetic metals.

Our starting point is to introduce a three-sublattice staggered potential into the fermionic SU(3) Hubbard model on the triangular lattice, which allows for the competition of the band insulator (BI) and Mott insulator (MI) phases at 1/3 filling. The Hamiltonian of the system reads

$$H = -t \sum_r \sum_{\delta} \left( \Psi_r^\dagger \Psi_r \right) + \frac{U}{2} \sum_r \Psi_r^\dagger \Psi_r \left( \Psi_r^\dagger \Psi_r \right) - \sum_r \Delta_r \Psi_r^\dagger \Psi_r ,$$

where $\Psi_r := (c_{r,0}, c_{r,1}, c_{r,2})$ is the SU(3) creation field operator with $c_{r,\alpha}^\dagger$ being the fermionic creation operator at the lattice position $r$ with the internal component $\alpha$, and $\delta$ stands for the nearest-neighbor (NN) vectors on the triangular lattice. The first two terms in Eq. (1) describe the three-component Hubbard model written in SU(3)-symmetric form, and the last term is a staggered potential which gives, respectively, the on-site energies $-\Delta$, 0, and $+\Delta$ to the three sublattices $A$, $B$, and $C$ of the triangular lattice, see Fig. 1(a). Fig. 1(b) dis-
plays the phase diagram of the model in the \( U-\Delta \) plane in units of the hopping parameter \( t \). Depending on the value of the staggered potential \( \Delta \), the BI phase is affected by the Hubbard interaction \( U \) in different ways. For \( 0 < \Delta \lesssim 6 \) the Hubbard interaction drives the BI into a paramagnetic metal (PM) and subsequently into a three-sublattice MI with a 120° pseudospin spiral order. For \( 6t \lesssim \Delta \lesssim 8t \) the Hubbard interaction destabilizes the BI into a charge-ordered magnetic insulator (COMI) at a first transition point. Interestingly, upon further increasing the Hubbard interaction, the broken SU(3) symmetry is restored and the system enters the PM. The transition into the MI phase occurs at a third transition point. For larger values of the staggered potential, \( \Delta \gtrsim 8t \), the PM is replaced by a charge-ordered magnetic metal (COMM) which separates the COMI from the MI phase. The BI, the COMI, and the MI phases are schematically depicted in Fig. 1(c). In the BI, all three fermionic components occupy mainly the sublattice \( A \), which has the lowest on-site energy. In the COMI, two components occupy the sublattice \( A \) and the third component resides on sublattice \( B \). In the MI phase, each sublattice is occupied with one component. In the limit \( U, \Delta \gg t \), the BI-to-COMI transition approaches the line \( \Delta \simeq 2U - 8t \) and the transitions from the COMI to COMM and from COMM to MI take place, respectively, at \( \Delta \simeq U/2 \) and \( \Delta \simeq U/2 - 2t \). This is in perfect agreement with the atomic limit results. The width of the COMM phase is finite for any finite value of \( t \).

The Hamiltonian (1) in the absence of the Hubbard interaction \( U \) reduces to a three-level problem in momentum space and represents a BI for any finite value of \( \Delta \). In order to investigate the ground state phase diagram of the Hamiltonian (1) we employed the dynamical mean-field theory (DMFT) technique which becomes exact in the limit of infinite dimensions [20]. The method is exact also in the non-interacting and in the atomic limit, and by fully taking into account local quantum fluctuations, it is a non-perturbative approach for studying the competition of charge and magnetic order in strongly correlated systems. We use the exact diagonalization impurity solver which enables us to compute local quantities with high accuracy, to directly access the real-frequency dynamical spectral functions, and to handle the large Hubbard \( U \) limit with no difficulty. We use the real-space DMFT method [21, 22] which we implemented for fermionic SU(\( N \)) systems in Ref. [23]. Due to the absence of electron-hole symmetry we add a chemical potential term to the Hamiltonian (1) and adjust it during the DMFT loop to achieve the desired 1/3 filling. We fix the inverse temperature to \( \beta = 20t \) and use 4-5 bath sites in our computations.

We have plotted the local density \( \langle c^\dagger \alpha \rho \rangle \) on the different sublattices \( A, B, \) and \( C \) and for the different internal components \( \alpha = 0, 1, 2 \) versus the Hubbard interaction \( U \) in Fig. 2 for the staggered potentials \( \Delta = 3t \) (a), \( \Delta = 7t \) (b), and \( \Delta = 10t \) (c). One can see from Fig. 2(a) that upon increasing the Hubbard interaction \( U \) from zero in the BI phase the particle density at the sublattice \( A \) decreases and the sublattices \( B \) and \( C \) get more populated. The system enters the PM at \( U \simeq 6t \), which is signaled by a finite density of states at the Fermi energy. Although the particle density on the different sublattices approach each other in this phase, they still remain different due to the finite staggered potential \( \Delta \) in the system. At \( U \simeq 12.5t \) the transition from the PM to the three-sublattice MI takes place. In the MI phase, the different components at each lattice site acquire different densities and each sublattice is mostly occupied with one of the three components, which leads to a 120° spiral order for the pseudospin vectors. For the stronger staggered potential \( \Delta = 7t \) in Fig. 2(b) the sublattice \( A \) is almost fully occupied at \( U = 0 \) and the particle density on this sublattice decreases upon introducing the Hubbard interaction \( U \). At \( U \simeq 9t \) there is a phase transition into the COMI. In this phase, two of the components show equal densities, which are large on sublattice \( A \).
We have distinguished the spectral functions at the different sublattices A, B, and C by the different colors blue, green, and red, respectively. The results are for 5 bath sites in the Anderson impurity problem.

The third component has a large density on sublattice B. The particle density on sublattice C is rather small. This phase obviously shows both magnetic and charge orders. Interestingly, the broken SU(3) symmetry in the COMI phase is restored again upon increasing the Hubbard interaction to $U \approx 16.5t$, where the system enters the PM. It is remarkable that the Hubbard interaction, at least in this particular problem, can have the effect of destroying long-range magnetic order rather than creating it. The transition from the PM to the MI phase happens at $U \approx 18.5t$. Although the PM-to-MI transition at $\Delta = 7t$ is sharper than the one at $\Delta = 3t$ it still seems to be continuous. Upon increasing the staggered potential from $\Delta = 7t$ to $\Delta = 10t$ in Fig. 2(c), the width of the COMI becomes larger, the PM gets substituted with a COMM, and the transition to the MI phase becomes discontinuous. The COMM shows both charge and magnetic orders and a finite density of states at the Fermi energy.

Next we discuss the single-particle spectral function, which is given in terms of the imaginary part of the single-particle Green’s function: $A_{\alpha\alpha}(\omega) = -\frac{i}{\pi} \text{Im} G_{\alpha\alpha}(\omega + i\epsilon)$, where $\epsilon$ is a small positive number. The spectral function is plotted in Fig. 3 for different paramagnetic (a) and magnetically ordered phases (b-c). For the paramagnetic phases PM and BI we have plotted the spectral function of only one component and for the magnetically ordered phases MI, COMI, and COMM the spectral functions of all three components $\alpha = 0, 1, 2$ are represented. In each panel of Fig. 3 we have distinguished the spectral functions at the different sublattices A, B, and C by the different colors blue, green, and red, respectively.

Fig. 3(a.1) depicts the spectral function in the PM for $(U, \Delta) = (9t, 0)$. Due to the absence of the staggered potential the spectral functions of the different sublattices are the same. We notice that for $\Delta = 0$ the Hamiltonian (1) reduces to the triangular lattice Hubbard model, which at 1/3 filling shows a transition from a PM to a three-sublattice MI at $U \approx 11t$. The larger spectral contribution above the Fermi energy $\omega = 0$ is due to the 1/3 filling. Keeping the Hubbard interaction $U = 9t$ and introducing the staggered potential $\Delta = 3t$ in Fig. 3(a.2), the system remains still metallic but spectral functions of different sublattices become different. For the sublattice $A$ the spectral contributions are transferred from above to below the Fermi energy by introducing $\Delta$, while for the sublattice $C$ it is the opposite. Fig. 3(a.3) shows the spectral function in the BI phase for the parameters $(U, \Delta) = (4t, 9t)$. The spectral function below the Fermi energy is dominated by the contribution from sublattice $A$; the contribution from sublattice $B$ is rather small and the contribution from sublattice $C$ is almost negligible. Right above the Fermi energy, there is a noticeable contribution from sublattice $B$. The high energy contributions belong mainly to the sublattice $C$. Such a spectral structure is expected, as the system is in the BI phase and there should be three well-separated bands due to the large staggered potential.

We have plotted the spectral function in the MI phase for the model parameters $(U, \Delta) = (22t, 7t)$ in Fig. 3(b).
Panels (b.1) to (b.3) correspond to the components $\alpha = 0$ to $\alpha = 2$. There is a Mott gap at the Fermi energy and the spectrum below the Fermi energy for each component is dominated by the contribution from one of the three sublattices. This is what one would expect as the system shows a three-sublattice magnetic order. The main low-energy peaks in Figs. 3(b.1) to 3(b.3) do not occur at the same energies: the peak originating from sublattice $A$ appears at much lower energies than the one originating from sublattice $C$. This energy difference is a result of the finite staggered potential in the system, which explicitly breaks the translational symmetry of the lattice and gives different on-site energies to the different sublattices. In the absence of $\Delta$, the peaks would have the same weight and occur at the same energies.

The spectral function in the COMI phase for $(U, \Delta) = (15t, 10t)$ is sketched in Fig. 3(c). The different panels correspond to the different components. The spectral functions of the two components $\alpha = 0$ and $\alpha = 2$ are the same and different from the spectral function of the component $\alpha = 1$. We observe that the spectral functions below the Fermi energy $\omega = 0$ for the two components $\alpha = 0$ and $\alpha = 2$ are largely governed by the contribution from sublattice $A$. The sublattice $B$ contains the major low-energy contributions of the spectral function for the third component $\alpha = 1$. The contributions of the sublattice $C$ to the spectral functions mainly lie above the Fermi energy. These results clearly support a phase which has both charge and magnetic order and a finite gap at Fermi energy. We have displayed the spectral function in the COMI for the parameters $(U, \Delta) = (23t, 10t)$ in Fig. 3(d). Again the different panels correspond to different components. There are contributions below $\omega = -15t$ mainly from sublattice $A$ and contributions above $\omega = +15t$ mainly from sublattice $C$, which can not be seen in the figure. Similar to the COMI, the spectral functions of the two components $\alpha = 0$ and $\alpha = 2$ are the same. The main part of the spectral function for all the three components is concentrated near the Fermi energy. There is a finite density of states at $\omega = 0$ and the system represents both charge and magnetic orders resulting in a COMM.

To summarize, multi-component systems have attracted a lot of attention in recent years due to their possible realization in optical lattices and the emergence of exotic states in the Mott regime [5–7, 19]. We have provided explicit evidence that multi-component systems also show interesting competition between charge and magnetic order, which has not been considered so far, neither experimentally nor theoretically. This is achieved by introducing a three-sublattice staggered potential to the fermionic SU(3) Hubbard model on the triangular lattice. We show that depending on the strength of the staggered potential, different intermediate phases separate the band insulator (BI) at weak and the Mott insulator (MI) at strong Hubbard interactions, resulting in a rich phase diagram. The fermionic SU(3) Hubbard model can be realized in optical lattices using $^6$Li [17, 18] or $^{173}$Yb [19], and the staggered potential can be created by using a superlattice which allows to adjust the depths of the three sublattices. The charge order can be probed by noise correlation measurements [24] and the magnetic order can be detected using a quantum gas microscope [25]. The excitation spectrum can also be measured using spectroscopic techniques such as radio frequency, Raman, and lattice modulation spectroscopy [2, 24, 26, 27].

We would like to mention that charge and spin order competition in two-component systems has been investigated extensively through the ionic Hubbard model (IHM) [28–31] and the Hubbard model with nearest-neighbor interaction [32–34]. The one dimensional IHM has recently been realized in optical lattices, and charge order [24] and different phase transitions [35] have been explored. For the two dimensional IHM, there are currently controversial theoretical predictions regarding the nature of the intermediate phase separating the BI and MI phases [36–38]. It will be subject to future research to take into account non-local quantum fluctuations and to search for new kinds of quantum states in multi-component systems, especially near the critical regions in the phase diagram 1(b). It would be also interesting to include spin-orbit coupling into the hopping term in Eq. (1) [39] and to study SU(3) topological phases with charge and magnetic order.

We would like to thank B. Irsigler and J. Panas for useful discussions. This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) via Research Unit FOR 2414 under project number 277974659. This work was also supported by the DFG via the high performance computing center LOEWE-CSC.

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