Quantum Monte Carlo Study of the Intermediate Phase in an Interacting Honeycomb Lattice with Staggered Potential

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By using the determinant quantum Monte Carlo method, we investigate the phase transitions in the ionic Hubbard model on the honeycomb lattice, varying the interaction strength and the difference in chemical potential on the two sublattices. Our exact numerical results reveal an interesting phase diagram where the electronic correlation may drive a band insulator metallic, and at a larger interaction, there is a second transition from metal to Mott insulator. It is also shown that the Mott insulating phase has antiferromagnetic long-range order at stronger interaction strength. A complete phase diagram is further achieved by studying the phase transition at large enough stagger potential and interaction strength, which shows that the intermediate state is more robust and occupies a large part of the phase diagram and that it should be more feasible to be detected experimentally.

Introduction—Correlation effects play an essential role in condensed matter physics, since many novel phenomena arise from these effects. A few examples include unconventional superconductivity[1, 2], fractional quantum Hall effect[3, 4], quantum spin liquid[5–7], and metal-insulator phase transitions[8, 9]. In the last decades, more correlated phenomena have been discovered, such as metal to charge-transfer insulator transitions in $\text{A}_x\text{CoO}_2$ (A=Na, Rb, K)[10], the evolution of electronic structure in SrRu$_{1-x}$Ti$_x$O$_3$[11], unconventional superconductivity in layered nitrides Li$_x$MNCI (M=Hf, Zr)[12], and possible exotic intermediate states between two or more competing phases[13]. Those phenomena are all relevant to the ionic Hubbard model[14].

The ionic Hubbard model contains the on-site Coulomb interactions and staggered potentials on bipartite lattices. There have been many analytical and theoretical studies on one-dimensional chains[14–17]. The study of this problem in the case of the one-dimensional lattice model of interacting bosons has already led to some interesting conclusions, where it is found that the competition between the on-site repulsion and the superlattice potential can produce a phase transition between a Mott insulator and a charge-density-wave insulator, with an intermediate superfluid phase[18, 19]. The Mermin-Wagner theorem prohibits long-range order in one-dimension, so any exotic phase would be present in higher dimensions. The Coulomb interactions give rise to a Mott insulating phase, while the staggered potentials favor a band insulating phase. Usually, novel phases appear in the intermediate region of two or more competing phases; thus, the investigation of the intermediate state between the two insulating phases is an fundamental problem of interacting many-body systems.

The seminal work of dynamical mean-field theory (DMFT) studies on a square lattice[13] suggests that an interaction-induced metallic phase exists in the intermediate region. Subsequently, cellular DMFT simulations have found a bond order phase[20] in this region, while determinant quantum Monte Carlo (DQMC) calculations of conductivity indicate a metallic phase[9]. More physical quantities, such as spectral function and magnetic structure factor, have been determined by DQMC to reconfirm the metallic phase[21]. In addition to metallic and bond order insulating phases, various other phases depending on the lattice geometry have been proposed on other bipartite lattices, such as semimetal[22] and half-metal[23]. Recently, exciting progress on ultracold atom experiments have been made, and the ionic Hubbard model could be realized in an optical honeycomb lattice[24]. Unfortunately, only the band insulating phase and Mott insulating phase were observed. Therefore, determining the existence of an intermediate phase or the nature of the intermediate phase is a subtle and largely open problem.

Motivated by the controversy and to stimulate further experiments, in this paper, we study the the ionic Hubbard model on a honeycomb lattice. Due to the novel properties in graphene-based materials[25, 26] and the discovery of topological states[27, 28], models defined on a honeycomb lattice are attracting increasing attention. By introducing interactions to those models with correlation effects considered, the models display exotic phases that have further enriched our understanding of physics far beyond the condensed matter community[29–31]. The ionic Hubbard model on a honeycomb lattice can not only be implemented in cold-atom systems but can also be realized on hydrogen graphene[32]; moreover, the new family of two-dimensional layered nitride materials Li$_x$MNCI (M=Hf, Zr) may be another candidate[12, 33]. It is natural and important to further investigate the possible intermediate state in the ionic Hubbard model on the honeycomb...
an electron with spin $\sigma$ of the system is characterized by the chemical potential $\mu$, respectively. The electron density hopping amplitude, on-site Coulomb repulsion, and $t$ where $A$ and $B$ sublattices, and the Hamiltonian is defined as

$$
\hat{H} = -t \sum_{i \in A, j \in B, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + H.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \Delta \sum_{i \in A, \sigma} \hat{n}_{i\sigma} - \Delta \sum_{i \in B, \sigma} \hat{n}_{i\sigma} - \mu \sum_{i \sigma} \hat{n}_{i\sigma} \tag{1}
$$

where $t$, $U$ and $\mu$ represent the nearest neighbor electron hopping amplitude, on-site Coulomb repulsion, and chemical potential, respectively. The electron density of the system is characterized by the chemical potential $\mu$. $\hat{c}_{i\sigma}^\dagger (\hat{c}_{i\sigma})$ is the operator that creates (annihilates) an electron with spin $\sigma$ at site $i$, and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$. Specifically, $\Delta$ is the staggered one-body potential between sites in A and B sublattices with opposite signs, which is also called the ionic potential. The band gap, $2\Delta$, has a nonzero value as a result of breaking the symmetry between sublattices A and B. We set $t = 1$ as the default energy level.

We adopt the exact DQMC method[34, 35] to study the phase transitions in the model defined by Eq.(1). DQMC is a powerful and reliable tool to investigate strong correlated electron systems. In the DQMC method, the partition function $Z = \text{Tr} \exp(-\beta H)$ is expressed as a path integral by the discretized inverse temperature $\beta$ over a set of random auxiliary fields. Then, the integration is accomplished by Monte Carlo techniques. The on-site interaction is decoupled by a Hubbard-Stratonovich (HS) transformation, which leads in a sum over the discrete HS field and leaves the Hamiltonian in a quadratic form in the fermion operators. The resulting quadratic form can be integrated analytically and thus comes out the Boltzmann weight, remaining as the product of the determinants of two matrices that depend on the HS spin variables. In the half-filled iron Hubbard model on the honeycomb lattice, the system is sign-problem free on account of the particle-hole symmetry, which allows us to achieve large $β$ simulations in order to converge to the ground state.

With the aim of exploring the phase transitions of the system, we compute the $T$-dependent DC conductivity, which is calculated from the wave vector $\mathbf{q}$- and the imaginary time $\tau$-dependent current-current correlation function[36] $\Lambda_{xx}(\mathbf{q}, \tau)$:

$$
\sigma_{dc}(T) = \frac{\beta^3}{\pi} \Lambda_{xx}(\mathbf{q} = 0, \tau = \frac{\beta}{2}), \tag{2}
$$

where $\Lambda_{xx}(\mathbf{q}, \tau) = \langle \hat{j}_x(\mathbf{q}, \tau) \hat{j}_x(-\mathbf{q}, 0) \rangle$, $\beta = 1/T$, $\hat{j}_x(\mathbf{q}, \tau)$ is the $(\mathbf{q}, \tau)$-dependent current operator in the $x$ direction. Eq.2 has been employed for metal-insulator transitions in the Hubbard model in many works and has already proved its validity[8, 36, 37].

We are also concerned about the magnetic properties of the system, and the antiferromagnetic (AFM) spin structure factor at wave factor $\bm{Q} = \bm{\Gamma}$ is

$$
S_{AFM} = \frac{1}{N_c} \langle \sum_{r \in A} \hat{S}_r^z - \sum_{r \in B} \hat{S}_r^z \rangle^2, \tag{3}
$$

where $N_c$ represents the unit cell number of the lattice, $\hat{S}_r^z$ is the $z$ component of the spin structure factor operator, and the angle brackets $\langle \cdots \rangle$ signify Monte Carlo simulations.

**Results and discussion**—We first calculate the temperature dependence of conductivity $\sigma_{dc}$ with
increasing interaction $U$ for a fixed value $\Delta = 0.3$. Basically, $d\sigma_{dc}/dt > 0$ at low $T$ indicates an insulating phase, while $d\sigma_{dc}/dt < 0$ at low $T$ corresponds to a metallic phase. In Fig. 1 (a), we can see that at $U = 0.0$ and $U = 1.0$, the $d\sigma_{dc}$ curve shows a concave down tendency and approaches the origin point as the temperature decreases. This kind of low $T$ behavior suggests that the system exhibits insulating behavior. Interestingly, the behavior becomes metallic as the on-site interaction increases to $U = 1.8$. A further increase in the interaction to $U = 2.5$ reinforces the metallic behavior, but the advance to $U = 4.5$ destroys the metallic state thoroughly and changes the system into a Mott insulator phase. When the staggered potential increases to $\Delta = 0.6$ for $U = 2.5$, it turns out that the increase in $\Delta$ suppresses the metallic behavior and that insulating behavior develops, which also implies that the value of $U = 2.5$ is not strong enough to drive the metallic phase for $\Delta = 0.6$.

We present more data in Fig. 1 (b) to emphasize the contrast and highlight the effect of the staggered potential. For $\Delta = 0$, at $U = 1.0$ and $U = 3.5$, $\sigma_{dc}$ increases as $T$ is lowered. When we calculated larger $U$ values ($U = 4.0$ and $U = 4.5$), $\sigma_{dc}$ decreases as $T$ is lowered, which shows insulator behavior when the staggered potential is absent. For the $U = 4.0$ case, the insulating phase at $\Delta = 0$ is displaced by a metallic phase when $\Delta = 0.6$.

Fig. 1 reveals one interesting phenomenon that the electronic correlation may drive a band insulator metallic, and at a larger interaction, there is a second transition from the metal to a Mott insulator. To further explore this issue, we plot the DC conductivity $\sigma_{dc}$ as a function of $U$ for fixed $\Delta = 0.3$ with five different temperatures in Fig. 2(b); Fig. 2(a) shows that the transition from metal to Mott insulator is restored at $\Delta = 0.0$ with a $U_c = 3.9$. The five curves shown in Fig. 2(b) intersect at two points, $U_{c1} = 1.4$ and $U_{c2} = 4.2$. In the range of $0 < U < U_{c1}$ and $U_{c2} < U < U = 5.0$, the conductivity $\sigma_{dc}$ values at higher temperature exceed those of lower temperature for the same $U$. The system maintains an insulating phase. The opposite situation emerges within the range of $U_{c1} < U < U_{c2}$. The conductivity increases as the temperature decreases, which demonstrates the metallic phase. The largest conductivity value for different $T$ values remains near $U_p = 3.0$. The two crosspoints represent the transitions from band insulator to metal to Mott insulator. Fig. 2(c) confirms these transitions with different $U_{c1} = 2.6$ and $U_{c2} = 4.3$ at $\Delta = 0.5$, and the largest conductivity occurs at approximately $U_p = 3.5$.

Interestingly, however, the position of the largest conductivity moves to larger $U$ as $\Delta$ increases, roughly following the law of $U_p(\Delta) = 2.5 + 2\Delta$, as that shown in Fig. 2(d). This result is quite different from that of the ionic Hubbard model on a square lattice, where the largest conductivity remains near $U_p(\Delta) = 2\Delta$, as one might expect from the $t = 0$ analysis[9]. In the Hubbard model on a square lattice, the charge density wave and local moments are perfectly balanced in the special $U = 2\Delta$ line at $t = 0$, and hence, the system is most likely to be metallic. At $t = 1$, the AFM point also lies on that line, which is $U_c = 0$ at $\Delta = 0$, but for a honeycomb lattice, the AFM point lies much higher above the line. Therefore, perhaps the AFM point “pulls” the largest sigma point up away from $U = 2\Delta$.

Fig. 3 provides the finite size scaling results of the AFM structure factor on lattices of size $L = 3, 6, 9, 12$, and $15$. If the third-order polynomial fitting curve of the data intersects the $y-$axis with a positive intercept, it indicates that a long-range AFM order exists. According to the simulation results shown in Fig. 3, we estimate that the critical point for $U$ is $U = 4.0 \sim 4.3$ when the band gap $\Delta = 0$, which is consistent with the previous studies of long-range AFM order[38]. As we can see, $\Delta$ suppresses the AFM structure factor, while $U$ plays an opposite role. An increase in the on-site interaction to $U = 4.5$ develops the long-range AFM order for $\Delta = 0.3$, and a further increase to $U = 5.0$ enables all calculated $\Delta$ values to exhibit a long-range AFM order.

In Fig. 4, we plot the conductivity $\sigma_{dc}$ as a function of the temperature for lattices up to $L = 15$ at metallic states (a) and insulating states (b). Both Fig. 4 (a) and (b) indicate that the lattice size has a distinct influence on the conductivity for $U \leq 3.0$. This result is
FIG. 3. (Color online) Finite size scaling results of the AFM spin structure factor $S_{AF}$, which is plotted as a function of $1/L$ for different staggered potential values at (a) $U = 4.0$, (b) $U = 4.3$, (c) $U = 4.5$, and (d) $U = 5.0$. The scattered symbols are our AFM calculation results. The curves represent the results of cubic polynomial data fitting. A positive and finite Y-intercept indicates that the long-range AFM order exists.

FIG. 4. (Color online) The conductivity $\sigma_{dc}$ is shown as a function of temperature at half-filling for various lattice sizes with $\Delta = 0.3$ of (a) metallic and (b) insulating states. Predictable because the finite size effects have remarkable impact on weak coupling. At $U = 3.0$ and $\Delta = 0.3$, there is an increase in $\sigma_{dc}$ with decreasing $T$ for the lattices that we have studied. Additionally, the metallic behavior weakens as the lattice size is increased. Although $\sigma_{dc}$ decreases with increasing lattice sizes, the signature of metallic behavior $d\sigma_{dc}/dt < 0$ is unchanged. At $U = 1.0$ and $\Delta = 0.3$, the system shows a insulating behavior at low temperature, and results on larger lattice sizes confirm this behavior. At larger interaction strength as $U = 4.5$ for the insulating states, the conductivity is almost independent on the lattice size.

In Fig. 5, we synthesize all the data and draw the emerging phase diagram, in which the phase boundaries are decided based on the temperature dependence of the conductivity $\sigma_{dc}$ and the finite size scaling of the AFM structure factor. This phase diagram has several key differences relative to previous models. First, the intermediate state that we found is more robust and occupies a larger part of the phase diagram. For example, at small $\Delta$, the intermediate phase disappears quickly as $U$ increases in the ionic Hubbard model on a square lattice, while here, the intermediate state is robust up to $U_c = 3.9$. Second, the critical $U_c$ is in a reasonable range for experimental detection. The phase transition in the Haldane-Hubbard model occurs at approximately $U_c = 11$, which is rather large for any exact numerical simulation of real materials. Furthermore, beyond previous results, we show a complete phase diagram where for large $\Delta$, the intermediate state disappears, and the system transitions from band insulator to Mott insulator directly.

Conclusions— Between the band insulating phase and Mott insulating phase, we find a metallic phase in the ionic Hubbard model on a honeycomb lattice. On a square lattice[9, 13, 21], Coulomb interactions produce an AFM insulating phase at infinitesimal $U$, and the competition with staggered potential induces a metallic phase[21]. By contrast, on the honeycomb lattice, a Mott insulator transition occurs at finite $U$, even without staggered interaction, and a rather wide region of $U$ and $\Delta$ for the metallic phase is found. In previous DMFT studies[22] on the honeycomb lattice, Ebrahimkhas and collaborators found that the intermediate phase is metallic. However, their phase boundaries are different from ours. The reasons for the difference are, on one hand, that they mainly focus on the nonmagnetic insulating phase, and, on the other hand, that in a
DMFT calculation, the correlations between clusters are considered through noninteracting bath sites. Our results are based on a more accurate numerical method, and neither the intercluster nor the intrachannel correlations are neglected.

In summary, we have studied the ionic Hubbard model on a honeycomb lattice by a determinant quantum Monte Carlo method. We found that the intermediate phase between the two insulating phases is metallic. The staggered potentials drive the metallic phase to the band insulating phase, while the effect of the Coulomb repulsion is different. The effect first drives the metallic phase into a nonmagnetic Mott insulating phase and then to the antiferromagnetic Mott insulating phase. As the Coulomb repulsion $U$ increases, the critical value of the staggered potential $\Delta_c$ increases, suggesting competition between the two energy scales. However, along the Mott metal insulator transition line, the effect of staggered potential is weak as the electrons are localized in the Mott insulating phase. Compared with previous theoretical proposals on some other models, our intensive numerical studies succeed in achieving a complete phase diagram, where the intermediate state is more robust and occupies a large part of the phase diagram, and it should be more feasible to be detected experimentally.

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