Cluster dynamical mean field theory of quantum phases on a honeycomb lattice

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We have studied the ground state of the half-filled Hubbard model on a honeycomb lattice by performing the cluster dynamical mean field theory calculations with exact diagonalization on the cluster-impurity solver. Through using elaborate numerical analytic continuation, we identify the existence of a ‘spin liquid’ from the on-site interaction $U = 0$ to $U_c$ (between 4.6$t$ and 4.85$t$) with a smooth crossover correspondingly from the charge fluctuation dominating phase into the charge correlation dominating phase. The semi-metallic state exits only at $U = 0$. We further find that the magnetic phase transition at $U_c$ from the ‘spin liquid’ to the Néel antiferromagnetic Mott insulating phase is a first-order quantum phase transition. We also show that the charge fluctuation plays a substantial role on keeping the ‘spin liquid’ phase against the emergence of a magnetic order.

Quantum phase transition is a fascinating physics subject, which describes an abrupt change of the ground state of a quantum many-body system tuned by a non-thermal physical parameter, often accompanied with a novel quantum emergence phenomenon. As a canonical quantum phase transition, the Mott transition, from metallic to insulating state tuned by electronic Coulomb interaction, is one of the most celebrated and difficult problems in condensed matter physics. The resultant insulating state, namely Mott insulator, usually adopts spontaneous symmetry breaking in two and three spatial dimension to form a long-range antiferromagnetic (AFM) order to release the spin entropy due to localized electrons. Theoretically, the simplest model to capture such physics is the standard one-band half-filled Hubbard model. In the large Coulomb interaction limit this model reduces to a standard Heisenberg model with an AFM order in its ground state.

Nevertheless, an insulating ground state without any spontaneous symmetry breaking, namely spin liquid, may arise if there is frustration. Actually the spin liquid is a genuine Mott insulating state in a sense that it is adiabatically separated from a band insulator. Spin liquid has been one of the most intriguing issues in condensed matter physics since it was introduced nearly forty years ago and continuously in intense research.

To help to clarify this issue, we performed the cluster dynamical mean field theory calculations for the half-filled Hubbard model defined on a honeycomb lattice as,

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the electron creation (annihilation) operator with spin $\sigma$ ($\uparrow$ or $\downarrow$) at lattice site $i$, $\langle ij \rangle$ represents the summation over the nearest neighbors, $t > 0$ is the nearest neighbor hopping integral, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ with the on-site Coulomb repulsion $U$.

Our calculated results are schematically summarized in Fig. 1. By the calculations, we show that a disordered phase of ‘spin liquid’ exists from $U = 0$ to $U_c$, at which it transforms into the Néel AFM insulating phase via a first-order quantum phase transition.

The dynamical mean field theory (DMFT) maps a quantum lattice model onto a single lattice site, a quantum impurity, dynamically coupled to a self-consistently determined bath of free electrons that represents the rest of the lattice. Thus the DMFT fully considers local quantum dynamical fluctuations, much beyond conventional mean-field methods. The DMFT has substantially improved our understanding on the nonperturbative properties of correlated electron systems, particularly the Mott transition. The cluster dynamical mean field theory (CDMFT) is a natural extension of the DMFT to include the missed short-ranged spatial correlations through a proper replacement of a single-site impurity by a cluster of lattice sites, which is constructed to reflect the lattice symmetry and local lattice structure.

FIG. 1: (Color online) Schematic phase diagram of the one-band Hubbard model on a honeycomb lattice at half-filling. $U_c$ is between 4.6$t$ and 4.85$t$.
features \cite{10,12}. The CDMFT has been successfully applied to study a variety of ordered phases, and opens an avenue to directly study quantum phase transitions.

Here it should be addressed that for the (C)DMFT the thermodynamic limit is naturally taken from the outset through a self-consistent procedure \cite{3,12}. As a nonperturbative approach to treat many-body correlation effects, the (C)DMFT works well in the whole coupling regime and becomes exact in the two contrary limits of both noninteracting and infinite-interacting cases. For finite-size quantum Monte Carlo simulations or exact diagonalizations, in contrast, the thermodynamic limit is extrapolated through finite-size scaling. Correspondingly, the CDMFT allows for spontaneous symmetry breaking, while the finite-size approaches have difficulty in finding a long-range order and related phase transition or underestimated ordered phases. Thus the CDMFT and finite-size approaches are complementary to each other, both of which together can give more conclusive results than they alone.

In CDMFT calculations, the target in the self-consistent procedure is to obtain a lattice imaginary frequency local Green’s function matrix $G_{ij}(\omega_n)$ (subscripts $i$ and $j$ being site indices of a chosen cluster) by assuming its self-energy matrix identified as the one of the corresponding cluster-impurity Green’s function matrix $G_{imp}(\omega_n)$, derived from the Dyson equation. In order to study a ground state, we apply exact diagonalization rather than quantum Monte Carlo simulation to solve a cluster-impurity model \cite{13,14}. Specifically, we employed the robust Krylov-Schur algorithm based SLEPc \cite{15} to accomplish the large-scale sparse matrix diagonalization efficiently and stably \cite{16}. Here we particularly emphasize that to carry out an elaborate numerical analytic continuation from an imaginary frequency Green’s function $G_{ii}(\omega_n)$ onto a real frequency retarded Green’s function $G_{ii}(\omega + i0^+)$ is crucial to unambiguously identify whether or not an energy gap exists at a small on-site interaction $U$ \cite{17,19}.

In such a way, the energy gap resolution can be achieved as high as $10^{-3}t$, which is hardly reached by other methods.

We first performed the CDMFT calculations for one-dimensional (1D) Hubbard model at half-filling with a cluster-impurity model respecting two and four lattice impurity sites, which serves as a benchmark for the further calculations. The calculated results are reported in Fig. 2 in quantitative comparison with the Bethe Ansatz exact solution \cite{20}. As we see, the two-site CDMFT result has been already in excellent agreement with the exact solution. Especially, by using the numerical analytic continuation, we can unambiguously identify a finite energy gap immediately develops once $U$ is nonzero. Thus the short-ranged spatial correlations play a dominant role in local spectral functions and properties even though the spatial correlations have long-ranged power-law behavior in 1D Hubbard model \cite{21}.

It is also well-known that the quantum fluctuations are much stronger in one-dimension than in higher dimensions. Hence it is highly expected that the higher dimensional CDMFT results are more reliable and encouraging than the one-dimensional ones.

Figure 3(a) schematically shows the cluster-impurity model constructed for a honeycomb lattice. Such a model reflects sixfold rotational symmetry and an impurity site with a lattice coordination number of 3, which are the essential features of a honeycomb lattice. We also add a direct link between each pair of the nearest bath levels so that we can include the propagation of an electron from one impurity site through the outside of the cluster (the bath) to any other impurity site in the calculations.

When the on-site interaction $U = 0$, the half-filled Hubbard model on a honeycomb lattice reduces to a set of free Dirac fermions with a linear DOS around the Fermi energy. As shown in Fig. 3(b), the numerical analytic continuation can well repeat the exact DOS. Particularly, around the Fermi energy both are the strictly same even though the DOS is not differentiable at the Fermi energy.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure2.png}
\caption{(Color online) Energy gap $\Delta$, namely single-particle spectral gap, as a function of the on-site interaction $U$ in the one-dimensional half-filled Hubbard model, calculated with the two-site ($N_c=2$) and four-site ($N_c=4$) clusters, respectively. The dashed curve denotes the exact one from the Bethe ansatz solution. The inset zooms in the small-$U$ dependence.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure3.png}
\caption{(Color online) (a) Cluster-impurity model configuration for a honeycomb lattice. Filled circles denote the impurity sites. Unfilled circles denote the bath levels. Links represent the hopping paths. (b) Density of states of the model when $U=0$. The blue curve is the exact one. The red one was obtained by the numerical analytic continuation.}
\end{figure}
In this study, we define the magnetization \( m = \langle n_i - n_{\bar{i}} \rangle / 2 \) on a site. Being bipartite, a honeycomb lattice can be divided into two sublattices \( A \) and \( B \). If a Néel AFM state appears, \( m \) will alternatively take positive and negative along with sublattices \( A \) and \( B \), namely being staggered magnetization. As we see from Fig. 4 when \( U < U_{c2} = 4.85t \), a paramagnetic solution of \( m = 0 \) is stable, namely no spin polarization on each site, but over \( U_{c2} \) this solution is no longer stable and \( |m| \) abruptly jumps over 0.2. On the other hand, when \( U > U_{c1} = 4.6t \) a staggered magnetization solution with \( |m| > 0.16 \) is stable, namely a Néel AFM phase takes over, but below \( U_{c1} \) \( m \) immediately plummets to zero. Between \( U_{c1} \) and \( U_{c2} \), these two solutions coexist. Such a hysteresis behavior indicates this magnetic transition is a first-order quantum phase transition.

We calculated the DOS for a small on-site interaction \( U \) with extreme caution through elaborate numerical analytic continuation \[18\]. The calculated DOS are then plotted in Fig. 5. Similar to the case of 1D Hubbard model, what we find is that there is also a definite energy gap opening at the Fermi energy once \( U \) is nonzero. In comparison with the case of \( U = 0 \) by checking the enclosed area, it is further shown that the corresponding states nearby the Fermi energy are clearly moved away from the gap rather than pushed to the two sides of the gap. To be specific, for \( U = 0.4t \), \( 0.8t \), and \( 1.2t \), the energy gap is found as small as \( \Delta = 2.5 \times 10^{-3}t \), \( 1.0 \times 10^{-2}t \), and \( 0.023t \), respectively. For a rather large \( U \), a relatively large energy gap opens with a substantial portion of states moved away from the Fermi energy into below \(-3t\) and above \(3t\), corresponding to the Hubbard band states. For a \( U \) further larger than \( U_{c2} \), the system transforms into the Néel AFM phase. The on-site spin degeneracy is then lifted. The spin-up (spin-down) resolved DOS at \( A \) sublattice is the same as the spin-down (spin-up) resolved DOS at \( B \) sublattice, as shown in Fig. 6.

Figure 7 shows the energy gap \( \Delta \) as a function of the on-site Coulomb interaction \( U \) on a honeycomb lattice. The inset zooms in the small-\( U \) dependence. Note that the energy gap is in linear \( U \)-dependence after the transition.
spin valence bond structures, spin anisotropic structures, and charge density waves. We can also exclude another possibility to break the translation symmetry that every six sites form a benzene-ring-like plaquette to further form a plaquette-singlet valence bond solid pattern in a honeycomb lattice. If such a pattern exists, the states nearby the Fermi energy will be pushed to the two sides of the gap rather than moved away. Thus this nonmagnetic insulating phase from $U = 0$ to $U_c$ (between $4.6t$ and $4.85t$) can be classified as a ‘spin liquid’ phase in the sense that it is tuned on by the on-site interaction $U$. 

To understand the underlying physics, we examine the double occupancy, defined as $D = \langle n_\uparrow n_\downarrow \rangle$ on a site. The ground state energy per site $E_g = \langle \hat{H} \rangle / N$ of Hamiltonian (1) is a function of the on-site interaction $U$. Its derivative is nothing but the double occupancy, namely $\partial E_g / \partial U = \langle n_\uparrow n_\downarrow \rangle$. Thus the double occupancy $D$ directly describes a quantum phase transition tuned by $U$. In Fig. 8 the $U$-dependence of the $D$ likewise shows a hysteresis behavior between $U_{c1}$ and $U_{c2}$. This means the energy level crossing in the ground state through the magnetic transition as $U$ increasing, being a characteristic of a first-order quantum phase transition [1].

The on-site interaction $U$ tunes or controls the Hamiltonian (1) through the double occupancy $D$. Moreover, the localization degree of an electron, as well as the local Dsonian (1) through the double occupancy $U$ on a honeycomb lattice, a small energy gap opening to tune the system into an insulating phase with a large double occupancy namely large charge fluctuation, as shown in Fig. 8. The calculations show that the small-$U$ induced energy gap is a consequence of the interplay between the zero-DOS at the Fermi energy (Dirac Cone band) and local charge correlation, not a conventional correlation-driven Mott insulating gap. On the other hand, the correlation effect will become dominating nearby the magnetic transition. Actually Fig. 8 has shown that the energy gap becomes a linear function of $U$ after the transition, which is the canonical behavior of a correlation-driven Mott insulator. Thus the ‘spin liquid’ states nearby $U = 0$ are of charge fluctuation dominating while those nearby $U_c$ are of charge correlation dominating, and corresponding to the ones found by the quantum Monte Carlo simulations reported in Ref. [6]. Nevertheless our calculations show that a smooth crossover connects these two contrary parts. Meanwhile it is also indicated that the charge fluctuation plays a substantial role on keeping the ‘spin liquid’ phase against the emergence of an AFM order.

In summary, we have performed the cluster dynamical mean field theory calculations, allowing for the spontaneous symmetry breaking, to study the ground state of the half-filled Hubbard model on a honeycomb lattice. We find that a ‘spin liquid’ exists from $U = 0$ to about $4.6t$, in which the system takes a smooth crossover correspondingly from the charge fluctuation dominating phase into the charge correlation dominating phase, then it further transforms into the Néel AFM Mott insulating phase via a first-order quantum phase transition.

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