Phase transition in the two dimensional ionic-Hubbard model

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Abstract

We employ the dynamical mean field approximation to study the effects of ionic potential (∆) and on-site electron correlation (U) on 2D square lattice. At half-filling when the staggered potential (∆) dominate and (U = 0), the system is in band insulator phase. We find competition between U and ∆ can suppress the gap to zero and stay zero within the metallic phase. By increasing U beyond $U_c(\Delta)$ the system enters metallic phase. Further increasing U open the gap again and another phase (Mott insulator) will be appeared. For $U > 0$ and $\Delta = 0$ the phase of system is Mott insulator.

Keywords: Dynamical mean field theory, Ionic-Hubbard Model

1. Introduction

There are many examples which the interactions could affected on phase transitions, such as Metal-Insulator (MI) transition [1, 2], semi metal-insulator transition [3]. A famous model exhibiting these interactions is the ionic Hubbard model (IHM) which includes a tight binding term, an on-site repulsion potential and a staggered potential that takes periodic magnitudes on neighbouring sites [4]. When the staggered potential dominates, a band insulator results. In a bipartite lattice, the substrate can include a sub-lattice symmetry breaking (by ionic potential $\Delta$) so the ground state of this system will be a band insulator. The interaction can suppress the gap in Band Insulators (BI) phase, by increasing repulsion interaction the energy gap would be creates again [5]. On the strongly correlated limit, when the Hubbard term dominates over ionic term in IHM, i.e. $U \gg \Delta$, the system goes to Mott insulator phase. In this limit, large $U$ imposed no-double-occupancy constraint. In higher dimensions, many theoretical and numerical works were published which investigate transition between Mott insulator and band insulator phases in Ionic Hubbard Model (IHM). Many groups have been employed the dynamical mean field theory (DMFT) [5, 6], detrimental quantum Monte carlo (DQMC) [7] and cluster

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dynamical mean field theory (CDMFT) [8] on IHM for studying the phase diagrams of mono layer of square lattice or bilayer [9]. We present results on the two dimensional square lattice by using ionic Hubbard model obtained with iterated perturbation theory (IPT) based on DMFT [5]. The DMFT approach have becomes some of the most powerful methods to study strongly correlated systems. In this method a problem should be solved: the interaction between a single site of a lattice hybridized to a bath; The bath of non-interacting electrons must be determined self-consistently. The DMFT is a powerful method [1] which is capable of handling ionic and Hubbard interactions in IHM. This approximation becomes exact in limit of infinite coordination numbers. For lower coordination number, the local self-energy (k-independent) becomes only an approximate description. Therefore the most significant drawback of this approximation is expected to be underestimation of the spatial quantum fluctuations [3, 10–12], hence the values of the critical phase transition parameters maybe overestimated [13]. But the overall picture emerging from a simple DMFT method is expected to hold even when more complicated methods are employed, such as CDMFT [14]. The DMFT were used in two dimensions Bethe lattice. The existence of metallic phase between the BI and MI phase has been proved [5]. By studying of bilayer Hubbard model we could find results same as IH Model. Because if the inter planar coupling was considered sufficiently large, it results a band insulator with a gap like a staggered potential, $\Delta$ [15]. This problem could be generalized to the heterostructure such as SrTiO$_3$ and LaTiO$_3$, studies on these materials was demonstrated a metallic phase appearing at the interface between a MI and BI phase [8]. In this manuscript, we first present the details of the IHM model and DMFT technique within IPT in section II, in Section III we describe the results and discussions of DMFT method and phase diagram vs $U$ and $\Delta$ potentials. We end this manuscript with conclusion in section IV.

2. Model and Method

The 2D ionic-Hubbard model on a bipartite (sub-lattices A and B) square lattice (SQL) is given by

$$H = -t \sum_{i \in A, j \in B, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - \Delta \sum_{i \in A} n_i + \Delta \sum_{i \in B} n_i + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i \sigma} n_{i\sigma} \quad (1)$$

where $t$ denotes the nearest neighbour hopping and $c_{i\sigma}^\dagger (c_{i\sigma})$ are the creation (annihilation) operator of electrons at site i with spin $\sigma$. $\Delta$ is the ionic staggered potential which alternates sign between sites in sub-lattice A or B. The number operator is $n_{i,\sigma}$ which determines the number of electrons at site i with projection of spin $\sigma$. The chemical potential is $\mu = U/2$ at half filling and $U$ designates the on-site electron-electron repulsion Hubbard potential. We take t as the energy unit through out this paper, we will consider the average filling factor $\frac{\langle n_A \rangle + \langle n_B \rangle}{2} = 1$.

In this model for $t > 0$ and non-interacting limit $U = 0$, a band insulator phase represents with energy gap, $E_{gap} = 2\Delta$. The sites $A(B)$ will have poten-
Figure 1: (Color online) The comparison between electrons occupancy on sites $A$ and $B$ in Bi and MI phase. The $A$ sites have lower potential than $B$ sites. (a) In band insulator the electrons choose doubly occupy lower bands. (b) In Mott insulator phase the electrons prefer to occupy only one site, $A$ and $B$.

trial, $-\Delta(\Delta)$, respectively. The electrons prefer to doubly occupy lower bands.

The average filling factors at half-filling is $\langle n_B \rangle = 2$, $\langle n_B \rangle = 0$. In other limit, for $U \gg \Delta$, the system goes to MI phase with $\langle n_A \rangle = \langle n_B \rangle = 1$ [10]. The flow equation methods predicted in the intermediate region at some energy scales the ionic and Hubbard potentials can cancel each other's effect [10]. From this point of view the tight-binding term dominate the nature of the ground state. Therefore we expect the intermediate phase to be a metal [3, 16]. Here we study the IHM using the DMFT approach [5]. To formulate the DMFT machinery, first we consider IH Hamiltonian on the square lattice in paramagnetic phase. The interaction Green’s function in the bipartite lattice are,

\[
G(\vec{k}, \omega^+) = \begin{pmatrix}
\zeta_A(\vec{k}, \omega^+) & -\epsilon(\vec{k}) \\
-\epsilon(\vec{k}) & \zeta_B(\vec{k}, \omega^+)
\end{pmatrix}
\] (2)

where $\vec{k}$ is the momentum vector in first Brillouin zone (FBZ), $\epsilon(\vec{k}) = \epsilon(k_x, k_y) = -2t(cos(k_x) + cos(k_y))$ is the energy dispersion for square lattice, and $\zeta_{A(B)} = \omega^+ + \Delta + \mu + \sum_{A(B)}(\omega^+)$ with $\omega^+ = \omega + i\theta^+$. The self-energy, $\sum_{\alpha}(\omega^+)$ in DMFT is local and and independent of $\vec{k}$. The matrix elements of the self energy is diagonal and the off-diagonal elements are zero. The local Green’s function of two sub-lattices can be written as, $G_{\alpha}(\omega^+) = \sum_{\vec{k}} G_{\alpha\alpha}(\vec{k}, \omega^+),$

\[
G_{\alpha}(\omega^+) = \zeta_{\bar{\alpha}}(\omega^+) \int_{-\infty}^{\infty} \frac{d\epsilon \rho_0(\epsilon)}{\zeta_{A}(i\omega_n)\zeta_{B}(i\omega_n) - \epsilon^2}
\] (3)

where for $\alpha = A(B)$, $\bar{\alpha} = B(A)$. The bare density of state can be obtained
for square lattice,

\[ D(\epsilon) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \delta(\epsilon - \epsilon(k_x, k_y)) \]

\[ = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \delta(\epsilon + 2t(\cos(k_x) + \cos(k_y))) \]

\[ = \frac{1}{2t\pi^2} \int_{0}^{\pi} dk_x \int_{0}^{\pi} dk_y \delta(\epsilon + \cos(k_x) + \cos(k_y)) \quad (4) \]

The Eq. 4 can be evaluated by using the property of delta function, introducing of dimensionless parameters \( \tilde{\epsilon} = \epsilon / 2t \) and the substitution \( \alpha = \cos(k_\alpha) \) where \( \alpha = x, y \), so the DOS becomes:

\[ D(\epsilon) = \frac{1}{2t\pi^2} \int_{-1}^{1} dx \int_{-1}^{1} dy \frac{\delta(\tilde{\epsilon} + x + y)}{\sqrt{(1 - x^2)(1 - y^2)}} \]

\[ = \frac{1}{2t\pi^2} \int_{0}^{\pi} dx \frac{1}{\sqrt{(1 - x^2)(1 - (\tilde{\epsilon} + x)^2)}} \quad (5) \]

The Eq. 5 can be evaluated numerically for these two intervals, \(-1 \leq x \leq 1\) and \(-1 \leq (\tilde{\epsilon} + x) \leq 1\). We first guess the initial filling factor and self-energy \( [5] \). Then we determine the host Green’s function from the Dyson’s equation \( G^{-1}_{\alpha}(\omega^+) = \frac{G_{\alpha} - 1(\omega^+) + \sum_{\alpha}(\omega^+)}{\omega^+} \). Afterwards, we solve impurity problem and obtain \( \sum_{\alpha}(\omega^+) = \sum_{\alpha}(G_{0\alpha}(\omega^+)) \). We use IPT method as impurity solver \( [5] \). The iteration in these steps continues until convergence is reached. We calculate the density of state by \( \rho_{\alpha}(\omega) = -\Im \text{Tr}[G_{\alpha}(\vec{k}, \omega^+)/\pi] \). From the particle-hole symmetry at half-filling we obtain \( \rho_A(\omega) = \rho_B(-\omega) \) for the DOS of two sub-lattice. The total DOS for square lattice is obtained via \( \rho(\omega) = \rho_A(\omega) + \rho_B(\omega) \).

### 3. Results and Discussions

In Fig. [2] we showed the DOS for three values of \( U \) at a constant \( \Delta = 0.1t \). This figure can covers the whole range of energies. For small values of \( U \) (\( U \leq U_{c1} \)) the spectrum has simple gap. By increasing \( U \) (\( U_{c1} \leq U \leq U_{c2} \)), the overall feature of the low energy spectrum changes and the DOS around \( \omega = 0 \) has singularity and the gap was closed. When \( U \) increases (\( U \geq U_{c2} \)) we could see the upper and lower Hubbard band appear, symmetrically. These Hubbard bands are shown in Fig. [3].

The DOS of square lattice in Hubbard model (\( \Delta = 0 \)) has Van-Hov singularity around the Fermi level. When the ionic potential (\( \Delta \)) was added, at \( U = 0 \) the energy gap is about \( E_{gap} \approx 2\Delta \), and two singularities was appear in both sides of gap. By increasing \( U \) in \( U_{c1} \leq U \leq U_{c1} \) interval the Van-Hov singularities moves towards lower energies. In \( U \geq U_{c2} \) interval singularities move towards higher energies. For more Discussions in the scale of energy gap we consider the
self energy of this system, $\sum_\alpha(\omega^+) = \sum_\alpha'(\omega) + i \sum_\alpha''(\omega)$, where shape of imaginary part of self energy can show insulating or metallic phase of systems [5, 10]. The $\sum''_A(\omega)$ vanishes around $\omega = 0$ in BI and MI phases, according to the Fermi liquid theory in metallic phase $\sum''_A(\omega) = \omega^2$ [5]. We show these results in Fig. 4.

The energy gap could be calculated in two methods, first through measurement the gap of DOS, second from the formula of $E_{gap}$, 

$$E_{gap} = Z|\Delta - U\delta n/2 + S|$$

(6)

Where $Z$ is independent of $\alpha$, $\delta n = \frac{\langle n_A \rangle - \langle n_B \rangle}{2}$ and $S = \int_{-\infty}^{\infty} d\omega \sum''_A(\omega)/\pi\omega$. As can be seen the gap depends on repulsion interaction, strongly [5]. In Fig. 5, the dots diagram obtained from the DOS and the open square with error bars obtained from Eq. 6. These two diagrams have excellent agreement with each other. But about error bars, these errors estimated from calculation errors in $\sum''(\omega \to 0)$. We increased the accuracy of the calculations and we used two methods in direct numerical integration. These error bars obtained from considering all these results.

By repeating the calculation for wide range of Hubbard potential and ionic potential, we can map out the phase diagram of the square lattice for ionic-Hubbard model. We could find interesting results different from phase diagram of honeycomb lattice [10]. For $\Delta \approx 0$, the only critical repulsion potential is $U_c \approx 0$. In the whole range of $U$, Mott insulator phase is dominate. By increasing the amount of $U$ in $\Delta \approx 0$ for honeycomb lattice the semi metal phase is overcome and Dirac cone linearization holds [10]. But in square lattice a little increasing in $U$ for $\Delta \approx 0$ can open the gap, this could be explained as the easiness the phase transition of Schrodinger electrons compared to Dirac

Figure 2: (Color online) The density of states for square lattice in IHM are plotted for $U = 0.0, 0.3t, 1.2t$ and $\Delta = 0.1t$. In this figure, the gap is appeared in insulator phases then disappeared in metallic phase.
Figure 3: (Color online) The density of states for square lattice in IHH are plotted for $U = 4.5t$ and $\Delta = 0.4t$. In this figure, the Hubbard bands appeared in both sides of $\omega = 0$.

Figure 4: (Color online) The Imaginary part of self energy for $\Delta/t = 0.2$ plotted vs $\omega$. The top and low panel are related to Band insulator and Mott insulator. The middle panel is related to Metallic phase.
Figure 5: (Color online) The energy gap for $\Delta/t = 0.4$ with two methods plotted vs $U$ in unit of $t$. The gap (dots) is plotted from DOS and curve with error bars (open square) obtained from Eq. 6. The error bars related to numerical errors in calculation of $\sum''(\omega)$ at small $\omega$.

Figure 6: (Color online) The phase diagram of IHM on the square lattice by DMFT(IPT) method. The metallic phase is between two insulator phases.

Our results on phase diagram of 2D square lattice (at $T = 0$) have good agreement with results obtained from determinant quantum Monte Carlo (DQMC) [5]. In Ref. [7], three phases BI, MI and Metal are predicted. Regardless of some differences in upper border in Fig. 6 and Fig. 2 of Ref. [7], the overall shape of borders between different phases are the same. The point $U \approx 0$, $\Delta \approx 0$ in phase diagram, is the separation point of three phases. But if temperature increased $e.g. k_B T = 0.01$, the phase diagram will be changed [17]. In Ref. [17] for $\Delta \approx 0$ and $0 < U < U_{c1}$, the 2D square lattice is in Metallic phase. Similar studies have been done on bilayer square lattice IHM with interesting results [18].
4. Conclusion

We studied the ionic-Hubbard model on 2D square lattice by IPT method. We calculated density of state, energy gap and self-energy at \( T = 0 \) conditions. Our results showed a metallic phase is between to insulator phases. For \( \Delta > 0 \) the system is in band insulator \((0 < U < U_{c1}(\Delta))\). By increasing \( U \) in \( U_{c1}(\Delta) < U < U_{c2}(\Delta) \) region the system show metallic character. Finally, for \( U > U_{c2}(\Delta) \) the correlations transform the metallic phase to Mott Insulator. The calculations showed by increasing \( \Delta \) the metallic region becomes wider.

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