Flow Equations for the Ionic Hubbard Model

Mohsen Hafez,1 S. A. Jafari*,2,3 and M. R. Abolhassani1

1Department of Physics, Tarbiat Modares University, Tehran, Iran
2Department of Physics, Isfahan University of Technology, Isfahan 84154-83111, Iran
3The Abdus Salam ICTP, 34100 Trieste, Italy

Taking the site-diagonal terms of the one-dimensional ionic Hubbard model (IHM) as $H_0$, we employ Continuous Unitary Transformations (CUT) to obtain a "classical" effective Hamiltonian in which hopping term has been integrated out. For this Hamiltonian spin gap and charge gap are calculated at half-filling and subject to periodic boundary conditions. Our calculations indicate two transition points. In fixed $\Delta$, as $U$ increases from zero, there is a region in which both spin gap and charge gap are positive and identical; characteristic of band insulators. Upon further increasing $U$, first transition occurs at $U = U_{c1}$, where spin and charge gaps both vanish and remain zero up to $U = U_{c2}$. A gap-less state in charge and spin sectors characterizes a metal. For $U > U_{c2}$ spin gap remains zero and charge gap becomes positive. This third region corresponds to a Mott insulator in which charge excitations are gaped, while spin excitations remain gap-less.

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INTRODUCTION

Ionic Hubbard model (IHM) has been used to study neutral-ionic transition in organic compounds [1] and understanding role of strong correlations in ferroelectricity of metal oxides such as BaTiO$_3$, KNbO$_3$, KTaO$_3$ [2], as well as some quasi-one-dimensional materials such as (TaSe$_2$)$_2$I, K$_{0.3}$MoO$_3$ [3]. IHM Hamiltonian includes an staggered one-body external potential in addition to the Hubbard Hamiltonian. The Hamiltonian for this model is as follows:

$$H = -t \sum_{i \sigma} (c_{i\sigma}^+ c_{i+1\sigma} + h.c.) + U \sum_i c_{i\uparrow}^+ c_{i\downarrow}^+ c_{i\downarrow} c_{i\uparrow} + \frac{\Delta}{2} \sum_{i \sigma} (-1)^i c_{i\sigma}^+ c_{i\sigma},$$

(1)

where $c_{i\sigma}$ ($c_{i\sigma}^+$) is the usual annihilation (creation) operator at site $i$ with spin $\sigma$, $t$ the nearest neighbor hopping amplitude, $U$ the on-site coulomb interaction parameter, and $\Delta$ a one-body ionic potential. This model has a very interesting phase diagram at zero temperature at half-filling. When $\Delta \ll U$ this Hamiltonian, like the usual Hubbard Hamiltonian, is transformed to the Heisenberg spin Hamiltonian [1, 5] that describes a Mott insulator. In the opposite limit $\Delta \gg U$, one can ignore $U$, and a Bogoliubov transformation gives a simple band insulator with gap $\Delta$. The limit $\Delta \gg \Delta$ is a many-body insulator, while the limit $\Delta \ll U$ is a one-body insulator. Hence this model is a basis to study the issues like matrix-element effects in optical spectra of band insulators, versus many-body insulators [6].

Apart from offering two entirely different insulating states, yet there remains interesting question of the intermediate phase: What is the nature of the ground state for $U \sim \Delta$? Researchers have used various methods such as exact diagonalization (ED) [2, 3], density matrix renormalization group (DMRG) [7, 8, 9], quantum Monte Carlo (QMC) [4, 10, 11, 12], dynamical mean field theory (DMFT) [13, 14, 15], etc. to study the properties of this model.

The nature of intermediate phase still remains controversial: Bosonization study of Fabrizio and coworkers [16] indicates an spontaneously dimerized phase, which is also supported by spin-particle transformation study of Batista and coworkers [17]. There are also other works supporting this scenario [7, 8, 11, 15]. On the other hand, there are studies showing that the intermediate phase is metallic [1, 4, 10, 13]. Brune finds a metallic transition point in between the band and Mott insulating states, with simultaneous bond order [9]. Craco et. al. in addition to metallic region, report on a coexistence phase between the band and Mott insulating states [14].

In this work, we employ the method of continuous unitary transformations or flow equations to study the half-filled one-dimensional IHM in zero temperature subject to periodic boundary conditions. CUT method is used to obtain a "classical" effective Hamiltonian for IHM. This effective Hamiltonian which is free of fermionic minus sign problem, provides a simple picture of the nature of excitations when interpreted in terms of the transformed ground state. Then for $L = 20$ sites and with $\Delta = 20$ (energies are in units of $t$) spin and charge gap are numerically calculated for different values of $U$. These calculations indicate two transition points. For $U < U_{c1}$, spin and charge gap are both positive, for $U_{c1} < U < U_{c2}$ both are zero and for $U > U_{c2}$ spin gap remains zero while charge gap becomes positive. Hence this the transformed effective Hamiltonian gives band insulator for small $U$ region ($U < U_{c1}$), Mott insulator for large $U$ regime ($U > U_{c2}$), and metal for the region in between.

ATOMIC LIMIT

In the limits $U \ll \Delta$ and $\Delta \ll U$, the model becomes easy to understand and gives band and Mott insulators, respectively. Yet, another interesting limit in which the phase dia-
cal degrees of freedom, we consider a zero momentum mode
shown in Fig. 1. Since this Hamiltonian contains purely lo-
end, we consider a unit cell in real space of the 1D lattice
by admixing them is absent here. Hence the problem reduces
the 1D chain. In part (a), a state with energy

\[ E[n_{i\sigma}] = \frac{\Delta}{2} \sum_{i\sigma} (-1)^i n_{i\sigma} + U \sum_i n_{i\sigma} n_{i\downarrow}, \]

where the Hamiltonian can be written solely in terms of classi-
cal (commuting) variables \( n_{i\sigma} \). In this sense, the atomic limit
corresponds to the classic limit of a quantum problem, and it
becomes much easier to analyze. Any configuration \( \{|n_{i\sigma}\}\) is an eigen-state of this Hamiltonian. The hopping term which
causes quantum fluctuations of various \( \{|n_{i\sigma}\}\) configurations by admixing them is absent here. Hence the problem reduces
to finding out the configuration with lowest energy. To this
end, we consider a unit cell in real space of the 1D lattice
shown in Fig. 1. Since this Hamiltonian contains purely lo-
cal degrees of freedom, we consider a zero momentum mode
\( k = 0 \) which corresponds to repeating this unit cell all over
the 1D chain. In part (a), a state with energy \( E_a = U - \Delta \)
per unit cell is shown, while the one in part (b) has energy
\( E_b = 0 \) per unit cell. For \( E_a < E_b \), i.e. \( U - \Delta < 0 \), state (a)
indicating a band insulator is stabilized, while for \( U > \Delta \), the
Mott insulating state with energy \( E_b \) is stabilized. At \( U = \Delta \)
these two states are degenerate, and hence in \( k = 0 \) mode, \( \uparrow \)
spin can freely move in the unit cell of Fig. 1. Therefore the
picture in the atomic limit is as follows: Eq. (2) describes a
Mott insulator for \( \Delta < U \) and a band insulator for \( \Delta > U \).
The transition line \( \Delta = U \) is a metal phase shrunk to a line.

The question we would like to address in this paper is, what
happens if we turn on the quantum fluctuations around the
Hamiltonian \( H \) by introducing a finite hopping \( t \)? It turns out
that CUT is a very suitable tool to investigate this strong cou-
pling problem. We advertise the result in advance: The inclu-
sion of the hopping \( t \) will renormalize \( U \rightarrow U(t, U, \Delta), \Delta \rightarrow
\Delta(t, U, \Delta), t \rightarrow \tilde{t} = 0 \), as well as generating new couplings.

**CONTINUOUS UNITARY TRANSFORMATIONS**

Flow equations approach or, CUT method \[18\] was intro-
duced independently by Glazek and Wilson \[19\], and Weg-
ner \[20\]. Since then, this method has been applied extensively
to study various models in condensed matter and high energy
physics. Some examples include, the Anderson model \[21\],
Lipkin model \[22\], mapping of the electron-phonon inter-
action to an effective electron-electron interaction \[23\]. Sine-
Gordon model \[24\], RKKY interaction \[25\], as well as non-
equilibrium dynamics of strongly correlated systems \[26\] and
an attempt for a unified description of Fermi and Luttinger
liquids in all energy scales \[27\].

In this method the Hamiltonian is transformed by a unitary
operator \( U(\ell) \) where \( \ell \) is a parameter between zero to infinity.
Flow equation for \( H(\ell) = U(\ell)HU(\ell) \) becomes,

\[ \partial_\ell H(\ell) = [\eta(\ell), H(\ell)], \]

where \( \eta(\ell) = \partial_\ell U(\ell).U(\ell) \) is an anti-Hermitian operator
called generator. Here \( U(\ell = 0) = 1 \), as at \( \ell = 0 \) transformed
Hamiltonian is equal to \( H \). Wegner suggested the following
generator \[20\]:

\[ \eta(\ell) = [H^d(\ell), H^r(\ell)], \]

where \( H^d(\ell) \) (\( H^r(\ell) \)) is diagonal (off-diagonal) part of the
Hamiltonian. With this choice for the generator, transformed
Hamiltonian flows towards a diagonal or block-diagonal form
in the \( \ell \rightarrow \infty \) limit. Mielke introduced another generator that
is specially useful for band matrices \[28\] and preserves the
band nature of the Hamiltonian matrix. In this section, we use
Wegner generator to obtain an effective Hamiltonian for IHM.

It is obvious from Eq. (3) that the flow equations without
any approximation is very hard to solve for Hamiltonians that
include interaction. In applying the flow equations to IHM we
use an approximation similar to the one used by Kehrein and
Mielke in the context of Anderson model \[21\]. We approxi-
mate \( H(\ell) \) as,

\[ H(\ell) = -t(\ell) \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + h.c.) + \frac{\Delta(\ell)}{2} \sum_{i\sigma} (-1)^i c_{i\sigma}^\dagger c_{i\sigma} \]

\[ + \frac{U(\ell)}{2} \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}^\dagger c_{i\sigma} c_{i\sigma} \]

\[ + V(\ell) \sum_{i\sigma} c_{i\sigma}^\dagger c_{i+1\sigma} c_{i+1\sigma} c_{i\sigma}. \]

with initial conditions \( t(0) = 1, \Delta(0) = \Delta, U(0) = U \)
and \( V(0) = 0 \). Physical motivation behind considering n.n.
Coulomb interaction \( V \) as follows \[8\]: In the simple phase
diagram shown in Fig. 1, for a fixed \( \Delta \), as one increases \( U \),
the ionicity \( n_B - n_A \) which is the population difference be-
tween \( A, B \) lattice sites, suddenly drops from 1 to 0 at \( U_{c2} = \Delta \). If
an attractive n.n. term \( V \) can be generated, it opens up an
intermediate phase in which the \( 0 < n_B - n_A < 1 \); i.e. the unit
cell gently looses its polarization with respect to the half-filled
background and turns into a Mott insulator.

In Eq. (5), the first term is taken to be off-diagonal and other
terms are diagonal. This choice resembles the strong coupling
perturbation schemes starting from the atomic limit. There
one usually has to organize the hopping processes into those
terms which change the double occupancy, and those which do
not \[5\]. But here we show that the inclusion of smallest

![FIG. 1: (Color online) Lowest energy configurations for (a) Perfect band insulator, (b) Perfect Mott insulator.](image-url)
amount of $\Delta$ makes it possible to renormalize the whole hopping processes to zero (Eq. 14).

Using equation (4). With this convention, the Wegner generator is obtained as:

$$\eta(\ell) = t(\ell)\Delta(\ell) \sum_{i}\sum_{\sigma} \{ (-1)^{i} \left( c_{i+1\sigma}^{\dagger} c_{i\sigma} - h.c. \right) \}$$

$$-t(\ell)U(\ell) \sum_{i}\sum_{\sigma\sigma'} \{ c_{i\sigma}^{\dagger} c_{i\sigma'} c_{i+1\sigma} - c_{i-1\sigma}^{\dagger} c_{i\sigma} c_{i+1\sigma} - h.c. \}$$

$$-t(\ell)V(\ell) \sum_{i}\sum_{\sigma\sigma'} \{ c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} - c_{i-1\sigma}^{\dagger} c_{i\sigma} - h.c. \} + c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - h.c. \}$$ (6)

To obtain the flow equations, we need to calculate the commutator of $\eta(\ell)$ and $H(\ell)$. To do so, we split $\eta(\ell)$ into three parts

$$\eta(\ell) = \eta_{1}(\ell) + \eta_{2}(\ell) + \eta_{3}(\ell)$$

where $\eta_{1}(\ell)$, $\eta_{2}(\ell)$, and $\eta_{3}(\ell)$ denote the first, second, and third terms in equation (6) respectively. Similarly, $H(\ell)$ in equation (5) has four terms

$$H(\ell) = H_{1}(\ell) + H_{2}(\ell) + H_{3}(\ell) + H_{4}(\ell)$$

where $H_{1}(\ell) \ldots H_{4}(\ell)$ correspond to four terms in Eq. (5). Therefore:

$$[\eta(\ell), H(\ell)] = [\eta_{1}(\ell), H_{1}(\ell) + H_{2}(\ell)] + [\eta_{2}(\ell), H_{1}(\ell)]$$

$$+ [\eta_{3}(\ell), H_{1}(\ell)] + \text{irrelevant terms}, \hspace{1cm} (9)$$

where "irrelevant terms" are newly generated couplings which are not similar to Eq. (5). The commutators are calculated as follows:

$$[\eta(\ell), H_{1}(\ell) + H_{2}(\ell)] =$$

$$2t^{2}(\ell)\Delta(\ell) \sum_{i}(1+i)^{i} \left( c_{i\sigma}^{\dagger} c_{i\sigma} + c_{i\sigma}^{\dagger} c_{i+1\sigma} + c_{i\sigma}^{\dagger} c_{i+2\sigma} + h.c. \right)$$

$$+t(\ell)\Delta^{2}(\ell) \sum_{i} \left( c_{i+1\sigma}^{\dagger} c_{i\sigma} - h.c. \right), \hspace{1cm} (10)$$

and

$$[\eta_{2}(\ell), H_{1}(\ell)] = t^{2}(\ell)U(\ell) \sum_{i\sigma\sigma'} \sum_{j\beta} \times$$

$$\left( [c_{i\sigma}^{\dagger} c_{i\sigma'} c_{i+1\sigma} c_{i+1\sigma'} + c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i\sigma'} c_{i+1\sigma'} + c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma'} + c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - h.c. \right)$$

$$- [c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} + h.c. \right) \hspace{1cm} (11)$$

First and third terms are irrelevant,while second and fourth terms respectively become

$$\left( c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} - c_{i\sigma}^{\dagger} c_{i+1\sigma} c_{i+1\sigma} c_{i+1\sigma} \right)$$

$$+ \text{irrelevant terms}.$$
PHASE TRANSITIONS

Ionicity

Fig. 1 represents two limiting case of the Hamiltonian (2). For the band insulator, where both electrons of spin ↑ and ↓ prefer the B sites with energy $-\Delta/2$, the unit cell is fully polarized. In the opposite limit of the Mott insulator, there is only one electron per site, and the unit cell polarization is polarized. In the opposite limit of the Mott insulator, there is only one electron per site, and the unit cell polarization is zero. Therefore we define the ionicity for IHM as $n_B - n_A$ where $n_B$ and $n_A$ are the density of electron in B and A sites respectively:

$$n_B = \frac{1}{N} \sum_{\sigma, i \in B} \langle \hat{n}_{i\sigma} \rangle \tag{23}$$

$$n_A = \frac{1}{N} \sum_{\sigma, i \in A} \langle \hat{n}_{i\sigma} \rangle \tag{24}$$

The ionicity for the IHM is depicted in Fig. 2. As can be seen in the figure, the ionicity is 1 for $U < U_{c_1}$, indicating a band insulating state. For $U > U_{c_2}$, the ionicity becomes zero, characterizing a Mott insulator. The intermediate region $U_{c_1} < U < U_{c_2}$ is characterized by $1 > n_B - n_A > 0$. This basic physics in contained in an attractive nature of the induced $V$ term in Eq. (22). Without this term, there is only one phase transition at $U_c = \Delta$ (Eq. 2). However, the renormalization process leading to generation of $V$ term, opens up an intermediate state allowing for the smooth decrease of the ionicity from 1 (Band insulator) to 0 (Mott insulator), by partially polarizing the unit cell.

In this picture the reduction in the degree of polarization of the unit cell to intermediate values facilitates the charge transfer between the two sites of each unit cell. Therefore the resulting intermediate state must be a metal.

To investigate the intermediate state further, we numerically calculate the charge and spin gaps for the IHM. Spin and charge gaps are calculated as follows [29]

$$\Delta_s = E_0(N\frac{N}{2} + 1, N\frac{N}{2} - 1) - E_0(N\frac{N}{2}, N\frac{N}{2}), \tag{25}$$

$$\Delta_c = \frac{E_0(N\frac{N}{2} + 1, N\frac{N}{2} + 1) + E_0(N\frac{N}{2} - 1, N\frac{N}{2} - 1) - E_0(N\frac{N}{2}, N\frac{N}{2})}{2} \tag{26}$$

where $E_0(N_1, N_1)$ is the ground state energy in a sector with $N_1$ ($N_1$) electron in spin up (down) state. Since the unitary transformations do not affect the level spacing, the spin and charge gaps defined above will be the same for effective Hamiltonian (22) as well as the original Hamiltonian (1). Fortunately the effective Hamiltonian (22) is classical and hence free of fermionic minus sign issues. Therefore the ground state energy $E_0(N_1, N_1)$ in each sector can be numerically calculated with straightforward algorithms.

In Fig. 3 we have plotted the spin and charge gaps versus $U$ for a fixed value of $\Delta = 20$. The numerical calculation is done for $L = 20$ lattice sites, subject to periodic boundary conditions.

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In Fig. 3 we have plotted the spin and charge gaps versus $U$ for a fixed value of $\Delta = 20$. The numerical calculation is done for $L = 20$ lattice sites, subject to periodic boundary conditions. This figure shows two transition points at $U_{c_1} = 19.7$ and $U_{c_2} = 20$. For $U < U_{c_1}$ spin and charge gap are positive and identical. The gaped charge excitations characterizes an insulating state. However, since the spin gap coincides with the charge gap, the resulting insulating state must be a simple band insulator. For $U_{c_1} < U < U_{c_2}$ spin and charge gap are both zero, characteristic of metallic states [4,10,13,14]. Finally, for $U > U_{c_2}$ charge excitations will become gaped, while spin excitations remain gapless. Low-energy spin excitations, with gaped charge excitation is characteristic of Mott insulators. This picture is in agreement with the one emerging from Fig. 2 according to which, $n_i \equiv \sum_{\sigma} n_{i\sigma} = 1$.

For $\Delta = 1$ the transition points occur in $U_{c_1} = 0.3$ and $U_{c_2} = 0.7$ and for $\Delta = 2$ in $U_{c_1} = 0.9$ and $U_{c_2} = 1.7$. The phase diagram depicting the intermediate metallic region is shown in Fig. 4. In absence of $t$ term, the metallic region
is characterized by line $U = \Delta$ in this case both $U_{c_1}$ and $U_{c_2}$ coincide and the metallic region shrinks to a line. However, inclusion of quantum fluctuations via $t$ term, induces an attractive $V$ term which eventually broadens the metallic line $U = \Delta$ into the narrow region shown in Fig. 4. In the limit $U, \Delta \gg t$ where the effective Hamiltonian reduces to the atomic limit, the intermediate region for a fixed $\Delta$ shrinks to zero and the metallic remains single point at $U_c = \Delta [10]$. Therefore the large $\Delta, U \gg t$ limit of the Fig. 4 is a line on which band insulating and Mott insulating phases are degenerate.

In the ground state $|\tilde{\Psi}_0\rangle = |\Psi_0(\infty)\rangle$ of (22), the quantum fluctuations are frozen. The ground state of the original fermions is given by $|\Psi_0\rangle = U(\infty)|\tilde{\Psi}_0\rangle$. When this transformation is applied, it is expected to restore the low-energy spin spectrum of the Mott insulating state, as well as the excitation spectrum of the resulting metallic state.

The question of whether the intermediate metallic state is a Fermi liquid, or non-Fermi liquid can be investigated by studying the dynamic correlation functions $\langle \Psi_0 | O_j(t) O_0(0) | \Psi_0 \rangle$. But since it is difficult to calculate $|\Psi_0\rangle$ of the original fermions, one can use the generator to set up flow equations for the observable $O_j$ to instead calculate the quantity $\langle \tilde{\Psi}_0 | \tilde{O}_j(t) \tilde{O}_0(0) | \tilde{\Psi}_0 \rangle$. As far as the calculation of static quantities such as various energy gaps presented in this paper is concerned, the way one does the unitary transformation will not be important. But for dynamic correlation functions in order to capture the incoherent features in the electronic structure of strongly correlated systems such as IHM, one needs to organize the hopping processes depending on whether they change the double occupancy or not [31, 32].

To summarize, we have presented a strong coupling treatment of the ionic Hubbard model within the CUT approach. This enabled us to map the IHM into an effective Hamiltonian containing only commuting variables $n_{ij \sigma}$. Getting rid of fermionic minus sing problems in this way, enables us to investigate the energetics of the model Hamiltonian, suggesting the phase diagram presented in Fig. 4.

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[31] S. Kehrein, private communication