GUTZWILLER APPROXIMATION FOR PARAMAGNETIC IONIC HUBBARD MODEL: ANALYTIC EXPRESSION FOR BAND–MOTT INSULATOR TRANSITION* **

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The ionic Hubbard model is a paradigmatic setup for studying the competition between band and Mott insulating behavior. Within the variationally exact in infinite dimensions Gutzwiller approximation, we derive a compact analytic expression for the phase boundary between the Mott and band insulators. While the method reproduces the expected band–Mott insulator phenomenology, it does not capture the correlated metallic state at finite staggered potential found, for example, in dynamical mean-field theory. This absence highlights that the metallic phase originates from incoherent Hubbard-band physics rather than Fermi-liquid behavior well captured by the Gutzwiller approximation. Our formulation establishes a concise variational framework for the ionic Hubbard model, with natural extensions to nonequilibrium setups and spin-exchange dynamics.

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1. Introduction

The Hubbard model is probably the simplest, yet remarkably rich, quantum mechanical platform for describing correlated electrons on a crystallographic lattice. Its continuous appeal within the condensed matter community stems, among others, from its ability to capture essential features of Mott physics.

At half-filling, the model hosts a Mott insulating state characterized by frozen charge degrees of freedom due to strong onsite Coulomb repulsion, while spin degrees of freedom remain active via antiferromagnetic exchange.

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** This work is dedicated to Professor Józef Spałek on the occasion of his 80$^{\text{th}}$ birthday.

As shown by Spałek in his derivation of the t–J model [1] and in later analyses, spin dynamics remain active even away from half-filling. The nontrivial role of correlations beyond the insulating regime, as described by the t–J model, is revealed by the emergence of unconventional superconductivity [2–4].

The Hubbard model is also very versatile, as seemingly small extensions to its pristine form allow us to analyze a quantum-mechanical description of various phenomena on the verge of Mott physics. This is the case for the Hubbard model enriched by a staggered potential on a bipartite lattice (*i.e.*, an ionic potential) that captures the band-to-Mott insulator transition [5–18], and thus in the past has been proposed to capture the ionic-to-neutral insulator transition in organic charge-transfer solids [19], and ferroelectric transitions in perovskites [20].

More recently, the model has been studied in the context of flat bands [21], cold-atom setups [22–24], topological properties of the dimerized (bond-ordered) phase (initially discussed in Ref. [5]) that may occur between the BI/MI phase boundary [25], and within the context of time-dependent phenomena [23, 26].

Despite this broad interest, applications of the Gutzwiller approximation (GA), a popular mean-field many-body tool, to the ionic Hubbard model remain limited [27, 28]. Here, we develop a neat formulation of the Gutzwiller approximation based on a general projector [29–31]. This formulation is ready to be extended to the non-equilibrium setup [31, 32], as well as to include spin-exchange physics in a variational manner [33, 34]. In this work, however, we restrict our analysis to the equilibrium and low-energy physics of charge degrees of freedom in the paramagnetic ionic Hubbard model.

With the use of GA, we have derived an analytic formula for the band–Mott insulator phase boundary. In contrast to dynamical mean-field theory analyses, which reveal a metallic phase at the band–Mott insulator boundary in infinite dimensions [12, 16], our approach does not reproduce this feature. We attribute its absence to the fact that the GA inherently describes only Fermi-liquid behavior, thereby missing incoherent effects responsible for the metallic state.

2. Model

The half-filled ionic Hubbard model describes electrons moving on a bipartite lattice under the influence of both a staggered potential and onsite Coulomb interactions. Its Hamiltonian is

$$\mathcal{H} = -t \sum_{\langle \boldsymbol{ij} \rangle \sigma} c^{\dagger}_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + \sum_{\boldsymbol{i}} \left(\frac{U}{2} (n_{\boldsymbol{i}} - 1)^2 + \Delta (-1)^{\boldsymbol{i}} n_{\boldsymbol{i}} \right) , \tag{1}$$

where $n_{\boldsymbol{i}} \equiv n_{\boldsymbol{i}\uparrow} + n_{\boldsymbol{i}\downarrow}$, and $(-1)^{\boldsymbol{i}\in A} = 1$ $(-1)^{\boldsymbol{i}\in B} = -1$ distinguishes the two sublattices. In this formulation, $t > 0$ represents the hopping integral between nearest neighbors, U is the onsite Coulomb repulsion, and Δ sets the amplitude of the staggered ionic potential alternating between the two sublattices. The model possesses a combined particle–hole and sublattice-exchange symmetry ($A \to B$), which enforces half-filling on average. Consequently, there is no explicit chemical potential term.

3. Gutzwiller approximation

In order to analyze the properties of model (1), we use an efficient formulation of the Gutzwiller approximation [29–31], in which we define a general local Gutzwiller projector as

$$\mathcal{P}_{\boldsymbol{i}} = \sum_{\Gamma} \frac{\Phi_{\boldsymbol{i}\Gamma}}{\sqrt{\prod_{\sigma} \left(n^0_{\boldsymbol{i}\sigma}\right)^{n_\sigma} \left(1 - n^0_{\boldsymbol{i}\sigma}\right)^{(1-n_\sigma)}}} |\boldsymbol{i};\Gamma\rangle\langle \boldsymbol{i};\Gamma| \,, \tag{2}$$

where local Fock states are defined as $|\boldsymbol{i};\Gamma\rangle = \prod_\sigma (c^\dagger_{\boldsymbol{i},\sigma})^{n_\sigma}|0\rangle$ *i.e.* $|\boldsymbol{i};\Gamma\rangle \in \{|0\rangle, |\uparrow\downarrow\rangle, |\uparrow\rangle, |\downarrow\rangle\}$. The Gutzwiller approximation, variationally exact only in the limit of infinite dimensions, is enforced by imposing the following constraints:

$$\begin{aligned} \mathrm{Tr}\left(\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{\Phi}_{\boldsymbol{i}}\right) &= 1 \,, \\ \mathrm{Tr}\left(\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{\Phi}_{\boldsymbol{i}}\hat{c}^\dagger_{\boldsymbol{i}\sigma}\hat{c}_{\boldsymbol{i}\sigma'}\right) &= n^0_{\boldsymbol{i}\sigma}\delta_{\sigma,\sigma'} \,, \end{aligned} \tag{3}$$

where hat denotes the matrix representation of the object in the $|\boldsymbol{i};\Gamma\rangle$ base. Conveniently, the expectation value under the Gutzwiller approximation of any local operator can be calculated as $\langle \mathcal{O}_{\boldsymbol{i}}\rangle = \mathrm{Tr}[\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{\mathcal{O}}_{\boldsymbol{i}}\Phi_{\boldsymbol{i}}]$. While implementing the first constraint is relatively straightforward, the second one needs to be treated with some care, and specifically, we enforce it here through Lagrange multipliers λ_i. Eventually, we can define an effective single-particle Hamiltonian as

$$\begin{aligned} \mathcal{H}_* \;=\; & -t \sum_{\langle \boldsymbol{ij}\rangle\sigma} \left(R^*_{i\sigma}R_{j\sigma}c^\dagger_{\boldsymbol{i}\sigma}c_{\boldsymbol{j}\sigma} + \mathrm{H.c.}\right) \\ & + \sum_{\boldsymbol{i}} \left[\frac{U}{2}\mathrm{Tr}\left[\hat{\Phi}^\dagger_{\boldsymbol{i}}(\hat{n}_{\boldsymbol{i}} - 1)^2\hat{\Phi}_{\boldsymbol{i}}\right] + \Delta(-1)^{\boldsymbol{i}}\mathrm{Tr}\left[\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{n}_{\boldsymbol{i}}\hat{\Phi}_{\boldsymbol{i}}\right]\right. \\ & \left. + \lambda_{\boldsymbol{i}}\left(n_{\boldsymbol{i}} - \mathrm{Tr}\left[\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{n}_{\boldsymbol{i}}\hat{\Phi}_{\boldsymbol{i}}\right]\right)\right] \end{aligned} \tag{4}$$

satisfying $\langle\mathcal{H}\rangle = \langle\mathcal{H}_*\rangle_0$ ($\langle ...\rangle_0$ denotes an expectation value with respect to the Slater determinant), and where

$$R^*_{i\sigma} = \frac{1}{\sqrt{n^0_{i\sigma}\left(1-n^0_{i\sigma}\right)}}\mathrm{Tr}\left(\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{c}^\dagger_{i\sigma}\hat{\Phi}_{\boldsymbol{i}}\hat{c}_{i\sigma}\right). \tag{5}$$

Given a particle–hole with an $A \to B$ shift symmetry of our Hamiltonian, and our interest in the paramagnetic state, we can write

$$\begin{aligned}
\hat{\Phi}_{\boldsymbol{i}\in A} &= \tfrac{1}{\sqrt{2}}\begin{pmatrix} \phi_0 & 0 & 0 & 0 \\ 0 & \phi_2 & 0 & 0 \\ 0 & 0 & \phi_1 & 0 \\ 0 & 0 & 0 & \phi_1 \end{pmatrix}, \\
\hat{\Phi}_{\boldsymbol{i}\in B} &= \tfrac{1}{\sqrt{2}}\begin{pmatrix} \phi_2 & 0 & 0 & 0 \\ 0 & \phi_0 & 0 & 0 \\ 0 & 0 & \phi_1 & 0 \\ 0 & 0 & 0 & \phi_1 \end{pmatrix},
\end{aligned} \tag{6}$$

and $\lambda_{\boldsymbol{i}\in A} = -\lambda_{\boldsymbol{i}\in B} = \lambda$.

At equilibrium, all ϕ_α parameters can be real, and thus we can make a further parameterization

$$\begin{aligned}
\phi_0 &= \sqrt{2}\sin\theta\cos\varphi\,, \\
\phi_2 &= \sqrt{2}\sin\theta\sin\varphi\,, \\
\phi_1 &= \cos\theta\,,
\end{aligned} \tag{7}$$

where it is enough to assume $\{\theta,\varphi\} \in \{0,\pi/2\}$. With the above, we automatically satisfy the first Gutzwiller approximation constraint (*cf.* (3)). Moreover, we have

$$\begin{aligned}
n_A &= \mathrm{Tr}\left(\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{\Phi}_{\boldsymbol{i}}\hat{n}_{\boldsymbol{i}\in A}\right) = |\phi_1|^2 + |\phi_2|^2\,, \\
n_B &= \mathrm{Tr}\left(\hat{\Phi}^\dagger_{\boldsymbol{i}}\hat{\Phi}_{\boldsymbol{i}}\hat{n}_{\boldsymbol{i}\in B}\right) = |\phi_1|^2 + |\phi_0|^2\,, \\
R_A &= R_{\boldsymbol{i}\in A\sigma} = \frac{1}{\sqrt{n_A n_B}}\left(\phi^*_0\phi_1 + \phi^*_1\phi_2\right) = R^*_B\,.
\end{aligned} \tag{8}$$

In the above, for the sake of clarity, we leave complex conjugations even if ϕ_α are real in equilibrium. Finally, the variational energy per lattice site, $\langle\mathcal{H}_*\rangle_0/N$, reads

$$E(\lambda,\varphi,\theta) = T(\lambda,\varphi,\theta) + \sin^2\theta\left(\frac{U}{2} + \cos 2\varphi(\lambda - \Delta)\right) \tag{9}$$

with $T(\lambda, \varphi, \theta)$ being the energy of the single-particle effective Hamiltonian. We assume a simple rectangular density of states $N(\epsilon) = 1/2W$, where W is half of the bandwidth, and a dispersion that has the property $\epsilon_{k+Q} = -\epsilon_k$, so that

$$T(\lambda, \varphi, \theta) = -\frac{1}{2W} \int_{-W}^{W} \mathrm{d}\epsilon \, \sqrt{R^4 \epsilon^2 + \lambda^2} \,, \tag{10}$$

where spin degeneracy is compensated by the integral over the whole Brillouin zone. The saddle point of the energy functional can be found by solving a set of differential equations

$$\left\{ \frac{\partial}{\partial \lambda}, \frac{\partial}{\partial \varphi}, \frac{\partial}{\partial \theta} \right\} E = 0 \,. \tag{11}$$

In that manner, the saddle-point solution can differentiate between three phases:

— band insulator ($\lambda > 0$ and $\theta > 0$);

— correlated metal ($\lambda = 0$ and $\theta > 0$);

— Mott insulator ($\theta = 0$).

The first issue that we can immediately resolve is that equations (11) cannot lead to the correlated metal state for non-zero Δ. At $\lambda = 0$, equations (11) do not lead to a contradiction only if $\theta = 0$. For that reason, apart from the limiting $U = 0$ case, our approach leads only to band or Mott insulating phases on the Δ–U plane, separated by the Brinkman–Rice (BR) transition line.

We solve equations (11) numerically and observe that near the BR transition, λ goes to zero much faster than θ. Due to the apparent singularity in the kinetic energy at the transition, in the following, we determine the transition line analytically. We do this by analyzing equations (11) for $\lambda = 0$ in linear order of small θ

$$\begin{aligned} \left.\frac{\partial E}{\partial \theta}\right|_{\lambda=0} &= \theta \big[U - 2(W + \Delta \cos 2\varphi + W \sin 2\varphi) \big] \,, \\ \left.\frac{\partial E}{\partial \varphi}\right|_{\lambda=0} &= \frac{\theta}{2} \big[\Delta \sin 2\varphi - W \cos 2\varphi \big] \,. \end{aligned} \tag{12}$$

From the above, it follows that near the transition:

$$\cot 2\varphi = \Delta / W \tag{13}$$

and, therefore, the critical interaction strength, U_c, for which the BR transition takes place, is determined by

$$U_c/W = 2(1 + \sqrt{(\Delta/W)^2 + 1}) . \tag{14}$$

If $\Delta = 0$, it follows (*cf.* Eq. (13)) that $\varphi = \pi/4$, and we restore the usual relation $U_c/W = 4$ for the BR transition in the Hubbard model. The resulting phase diagram is presented in Fig. 1.

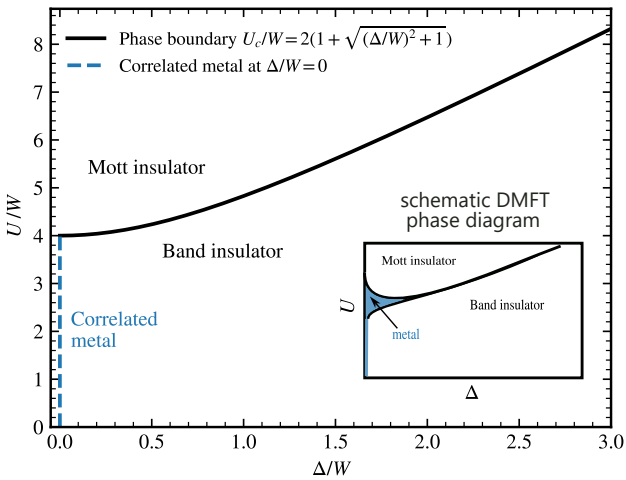

Fig. 1. Phase diagram in the $(\Delta/W, U_c/W)$ plane. The solid line denotes the phase boundary between the Mott insulating and band insulating states, given by $U_c/W = 2\left(1 + \sqrt{(\Delta/W)^2 + 1}\right)$. At $\Delta/W = 0$, the system exhibits a correlated metallic phase up to $U_c/W = 4$. The region above the boundary corresponds to the Mott insulator, while the region below corresponds to the band insulator. In the inset, we provide a schematic phase diagram obtained from dynamical mean-field theory as in Ref. [12].

4. Discussion

The Gutzwiller approximation is a many-body approach that becomes variationally exact in the limit of infinite dimensions. Although it does not capture high-energy quantum fluctuations responsible for spin exchange [33], it provides a good description of Fermi-liquid behavior. This is achieved primarily through its treatment of quasiparticle renormalization and the shift in chemical potential, both arising from the low-energy expansion of the real part of the self-energy. Moreover, the method successfully captures the freezing of charge degrees of freedom with increasing correlations, signaling the metal–Mott insulator transition, deemed the Brinkman–Rice transition.

As expected, our approach reproduces the phenomenology of the band-to-Mott insulator transition on the Δ–U plane, well established for the infinitely dimensional Hubbard model [12] (*cf.* Fig. 1). However, given its ability to describe Fermi-liquid behavior, it is somewhat surprising that, by construction, our approach does not yield a correlated metallic state for nonzero Δ in the vicinity of the band-to-Mott insulator transition [12, 16].

This observation, however, further illustrates [18] that the origin of the metallic phase is not of the Fermi-liquid type. Instead, it is rooted in incoherent features and interplay between Hubbard and ionic bands splits, which near the transition, result in the nonzero spectral function at the Fermi level.

5. Summary

In this work, we have analyzed the half-filled ionic Hubbard model within the Gutzwiller approximation, focusing on the competition between band and Mott insulating phases. By constructing a compact variational formulation based on general local projectors, we derived an analytic expression for the phase transition line separating the two insulating regimes. Our analysis shows that, while the Gutzwiller method correctly reproduces the expected band–Mott insulator phenomenology, it does not support the existence of a correlated metallic phase at finite staggered potential that has been observed via dynamical mean-field theory [12, 16]. Given intrinsic Fermi-liquid character of the GA, neglecting incoherent features related to Mott physics, we attribute the emergence of the metallic phase in the vicinity of the phase boundary between different insulators to the presence of spectral features of Mott–Hubbard bands. Our results, in the broad picture, highlight the complementary roles of different many-body approaches. Moreover, the formulation itself is readily extendable to nonequilibrium setups [31, 32] and to variational treatments of spin-exchange physics [33, 34].

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