
Physics Area - PhD course in
Theory and Numerical Simulation of Condensed
Matter

Unconventional Properties of Mott Insulators from the Ghost Gutzwiller Approximation

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Abstract

This Thesis demonstrates that an accurate description of a symmetry-invariant single-band Mott insulator within the ghost-Gutzwiller approximation necessitates the existence of in-gap single-particle modes that are strictly pinned at the chemical potential and carry no spectral weight in the physical single-particle excitation. Throughout the Thesis, we have endeavored to demonstrate that these zero-weight modes, rather than being a mere technical artifact of the variational construction, behave as genuine hidden quasiparticles, with measurable consequences whenever the insulator is perturbed, and which can be legitimately regarded as the sought-after Anderson's spinons.

Two case studies substantiate this claim. First, at the interface between a paramagnetic Mott insulator and a metal, these spinons reacquire charge and thereby spectral weight, hybridize with the metal and form heavy-fermion bands confined to a surface layer whose depth diverges with a mean-field critical exponent on approaching the Mott transition. This behavior is consistent with photoemission evidence of ambipolar in-gap states induced by surface doping of Ca_2RuO_4 .

Second, we have demonstrated that the symmetry-invariant Mott insulator stabilized within the ghost-Gutzwiller approximation exhibits a paramagnetic response in the presence of a Zeeman spin-splitting field. Remarkably, the spin magnetization m is carried entirely by the zero-weight modes, while the Hubbard bands remain unpolarized. The quadratic rise of the total energy, $E(m) - E(0) \sim m^2$, suggests that these hidden quasiparticles indeed possess a bandwidth that becomes the antiferromagnetic exchange $J = 4t^2/U$ in the strong coupling limit, as expected for the spinons.

Conversely, when symmetry is allowed to spontaneously break, and the single-band model allowed to become the expected antiferromagnetic insulator, the above exotic insulator gives way to a more conventional Hartree-Fock-like band insulator. Nevertheless, we can still stabilize antiferromagnetic solutions with tunable deviation from the Hartree-Fock limit, quantified through the local mutual information, which might better represent realistic antiferromagnets where quantum fluctuations are not negligible.

Taken together, these results demonstrate the ghost-Gutzwiller approach as a feasible variational method to explore the hidden excitations of Mott insulators, paving the way for future research into their unique properties.

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Publications

- [1] Antonio Maria Tagliente, Carlos Mejuto-Zaera, and Michele Fabrizio, *Phys. Rev. B* **111**, 125110 (2025)
- [2] Ivan Pasqua, Antonio Maria Tagliente, Gabriele Bellomia, Bartomeu Monserrat, Michele Fabrizio, and Carlos Mejuto-Zaera, Band-structure picture for topology in strongly correlated systems with the ghost Gutzwiller ansatz, *Phys. Rev. B* **113**, 155133 (2026)
- [3] Antonio Maria Tagliente, Ivan Pasqua, Michele Fabrizio, Direct minimization versus iterative embedding in the ghost-Gutzwiller method: a comparative study of magnetism in Mott insulators, *arXiv:2607.27156*

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1 | INTRODUCTION

In this chapter, we will provide a brief overview of the main concepts and motivations behind this Thesis, as well as of the most significant results that have been obtained.

Strongly correlated electron systems remain one of the richest sources of new physics in condensed matter, hosting exotic phenomena such as high-temperature superconductivity, quantum spin liquids, and topological phases of matter with fractionalized excitations. The novel physics displayed by these systems typically stems from the emergence of collective degrees of freedom that cannot be resolved within a single-particle picture. This poses a genuine theoretical challenge: a satisfactory description must capture the relevant many-body physics while remaining computationally tractable and, ideally, retaining a transparent physical interpretation.

One of the most successful approaches to this problem is dynamical mean-field theory (DMFT) [4], which has enabled a detailed understanding of a wide range of correlated phenomena, most notably the Mott metal-insulator transition. DMFT becomes exact in the limit of infinite spatial dimensions, or equivalently infinite lattice coordination number [5, 6], but still provides a very sensible approximation even for finite coordination lattices. However, this method encounters difficulties in describing symmetric phases whenever the true low-temperature phase spontaneously breaks a symmetry of the Hamiltonian.

An example relevant to the current thesis is that of a Mott insulator which exhibits emerging local magnetic moments. At low temperature, the entropy associated with these magnetic moments needs to be quenched. In general, quenching is achieved through magnetic ordering. However, if the Hamiltonian contains a sufficient degree of frustration and quantum fluctuations, the system fails to order down to zero temperature, resulting in what is known as a quantum spin liquid. Since such a circumstance is hardly feasible in a lattice with infinite coordination number, one could still attempt to describe a putative spin-liquid state by forcing the $O(3)$ symmetry associated with the local moments. The hope is that the state realized by forcing this symmetry is not merely a collection of free moments but exhibits the strong entanglement that characterizes a spin liquid. Unfortunately, this expectation

does not occur in DMFT, where the low-temperature state turns out to have the massive entropy of free local moments.

Spin liquids are typically studied using effective spin Hamiltonians derived from parent Hubbard-like models in the strong-coupling limit. These spin Hamiltonians inherently neglect charge degrees of freedom, assuming them to be completely frozen. This approximation is justified because the charge is locked at a much higher energy scale than the one governing spin dynamics. However, this seemingly reasonable approximation may fail to describe even low-energy physics in specific circumstances where the interplay between low-energy spin degrees of freedom and high-energy charge ones becomes significant. In such situations, methods that can describe both degrees of freedom on a similar footing are required. Therefore, even though DMFT fails to describe spin-liquids, simple methods are still desirable for hypothetical quantum spin liquids in high-coordination-number lattices where Mott localization of electron charge can be accessed more easily, and thus also its interaction with spin degrees of freedom. An example we will discuss in detail is the interface between a spin liquid insulator and a simple metal. In this case, and similar to the celebrated Kondo effect, the weak contact with the metallic bath drives the conversion of spins residing in a surface layer of the spin liquid insulator into in-gap heavy-fermion quasiparticles.

Gutzwiller projected wavefunctions have been extremely successful in classifying spin-liquid states [7, 8] and offering effective mean-field like descriptions. In this Thesis, we demonstrate that even the above mentioned interplay between charge and spin degrees of freedom can be successfully described employing Gutzwiller-like wavefunctions. Specifically, we employ the so-called *ghost* extension of the Gutzwiller wavefunction treated within the Gutzwiller approximation [9]. Just like DMFT, the ghost-Gutzwiller approximation becomes exact in infinite-coordination-number lattices, where it therefore provides strictly variational bounds on the total energy in excellent agreement with the exact DMFT results [9–12]. We remark that the connection between DMFT and the ghost Gutzwiller approximation has recently been strengthened by the demonstration that the ghost Gutzwiller approximation becomes equivalent to DMFT in the limit of infinitely many ghost orbitals [13], and its versatility has enabled applications to a broad range of phenomena [14–25].

However, this method, being rooted in the variational principle, allows constraining the solution into high-symmetry subspaces, even if they do not contain the ground state, thus overcoming the DMFT difficulties.

The conventional Gutzwiller variational wavefunction comprises an uncorrelated wavefunction, a Slater determinant or BCS wavefunction, acted upon by local linear

operators that diminish the weights of local configurations which incur substantial interaction energy. Both uncorrelated wavefunction and linear operators are determined variationally by minimizing the expectation value of the Hamiltonian, which is calculated through the Gutzwiller approximation.

The fundamental characteristic of the ghost-Gutzwiller wavefunction is that the uncorrelated wavefunction is defined within an auxiliary Hilbert space that is larger than the physical one. Consequently, the local linear operators serve as mappings from the local expanded Hilbert space to the local physical space and, accordingly, the physical fermion maps onto a weighted sum of the auxiliary fermions governed by a non-interacting Hamiltonian whose ground state is the uncorrelated wavefunction.

In correlated metals, the high-energy auxiliary fermions represent incoherent Hubbard bands, while the low-energy fermions represent coherent quasiparticles. Their weight vanishes as the system approaches the Mott transition. However, beyond the transition, these zero-weight modes, pinned at the chemical potential, are not redundant in describing the Mott insulator. Instead, they are crucial for enforcing the symmetries that would be spontaneously broken in the actual ground state, as we have demonstrated.

Initially, the role of the zero-weight auxiliary fermion, although significant, could be merely interpreted as a technical trick to prevent symmetry breaking in the ghost-Gutzwiller approach. Despite this, we discover compelling evidence that these fermions possess a physical significance, effectively functioning as concealed quasiparticles. These quasiparticles remain invisible in the single-particle spectrum, and yet affect observable quantities.

In fact, the Mott gap, long regarded as a featureless void in the single-particle spectrum, has recently emerged as a host of hidden low-energy structures. Within the framework of Green's functions, the gap of a Mott insulator, in stark contrast to that of a band insulator, is traversed by bands of Green's function zeros. When one of these bands crosses the chemical potential, it forms a so-called Luttinger surface, which is the locus of the roots of $\det G(0, \mathbf{k})$, where $G(\omega, \mathbf{k})$ represents the single-particle Green's function, as opposed to the Fermi surface, which is the locus of the poles. The existence of a Luttinger surface has been proposed to imply the presence of Landau's quasiparticles that carry no spectral weight [26–28], and it has been suggested to account for the violation of Luttinger's theorem [29, 30]. Even when these bands of zeros do not cross the chemical potential, they can still possess physical content. For instance, they may contribute to the Green's function winding number [31], which is a topological invariant. In that case, they fulfill bulk-boundary correspondence [32] leading to neutral spin-1/2 edge modes [33].

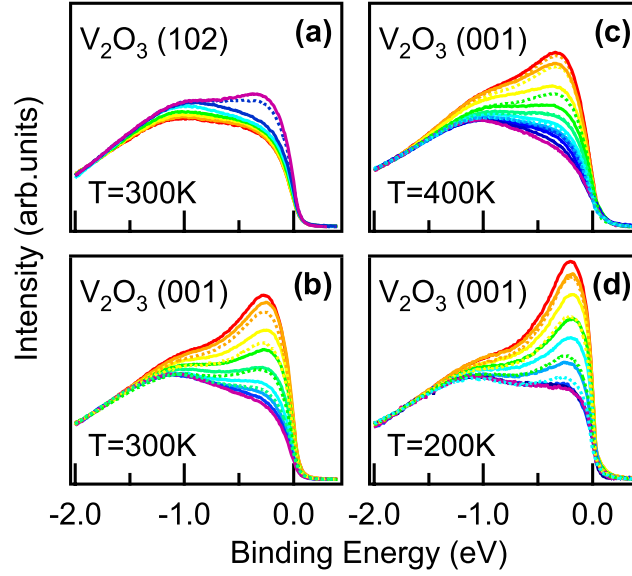


Figure 1: Plot of photoemission intensity for a sample of vanadium sesquioxide cleaved along the (102) (panel a), and the (100) plane (panels b,c,d) and different temperatures. The colors correspond to different photoemission angles, from normal (red) to grazing (violet). From reference [43].

It is therefore intriguing to identify the auxiliary fermions that lose their spectral weight entering the Mott insulating phase with the hidden structures that populate the Mott-Hubbard gap.

This is precisely the scope of this thesis. In particular, we will examine two case studies involving single-band models to investigate this issue: an interface between a metal and a paramagnetic Mott insulator [1], and a Mott insulator that breaks spin $SU(2)$ symmetry, either explicitly or spontaneously [3].

In the next chapters we discuss in detail our results. In what follows we just briefly outline the main findings.

1.1 Fate of spinons at the interface with a metal

Interfaces and surfaces provide a precious, and experimentally accessible, window on the physics of strongly correlated electron systems [34–40]. An example is provided by the evidence in photoemission that the expected quasiparticle peak in the correlated metal phase of V_2O_3 is actually severely suppressed across an entire surface layer [41–43] (Fig. 1).

Theoretical work based on inhomogeneous DMFT [45–48] and on the Gutzwiller variational approach [44, 49], applied to prototypical slab and junction geometries,

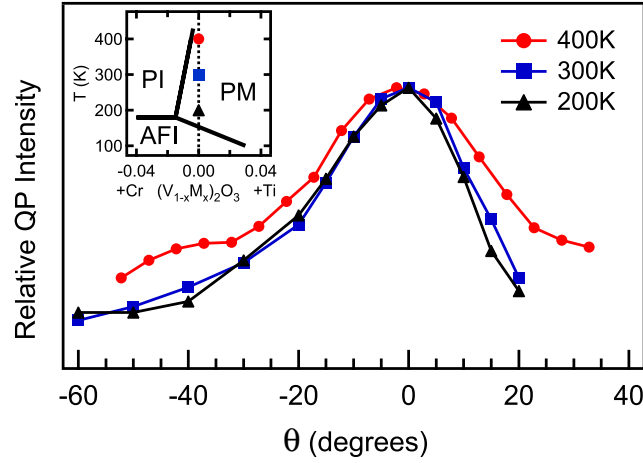


Figure 2: Photoemission evidence for a quasiparticle dead layer at the surface of metallic V_2O_3 : angular attenuation of the quasiparticle weight extracted from the spectra of Fig. 1, at three points of the phase diagram (inset). The attenuation length exceeds the structural surface region and increases on approaching the Mott transition, consistent with the diverging correlation length ξ predicted by Gutzwiller calculations [44]. Reproduced from Ref. [43].

established that a strongly correlated metal, unlike an ordinary Fermi liquid, possesses an intrinsic electronic length scale beyond the Fermi wavelength, which is associated to the distance from the Mott transition. Indeed, it was shown that the quasiparticle weight $Z(\ell)$ as function of the distance ℓ from the surface heals exponentially over a correlation length $\xi \propto (U_c - U)^{-\nu}$, with mean-field exponent $\nu \simeq 1/2$, which diverges at the Mott transition $U = U_c$. This single length scale unifies seemingly disparate phenomena: the evanescent penetration of metallic quasiparticles into a Mott insulating barrier [47–49] and the anomalously thick dead layer of suppressed metallicity beneath the surface of V_2O_3 , whose extent grows on approaching the Mott transition [43] (Fig. 2).

These results established correlated heterostructures both as a diagnostic tool, turning surface-sensitive spectroscopy into a probe of Mott criticality, and as a design platform, in which interfacial proximity becomes a control parameter for correlated phases on the same footing as pressure or doping.

We have studied an interface between a paramagnetic Mott insulator and a metal. First we employed the conventional Gutzwiller wavefunction in which the dimensions of the physical and auxiliary Hilbert spaces are the same. The Hamiltonian is intentionally not particle-hole symmetric, in which case both conventional Gutzwiller approximation and DMFT predict a first order Mott transition even at $T = 0$. This presents an opportunity to extend the findings of Borghi et al. [44] to the context of bulk first-order phase transitions. Remarkably, even in this scenario, we could derive a description in terms of critical phenomena, specifically of a wetting

transition.

Next, we applied the ghost-Gutzwiller approximation with three auxiliary fermions per physical one. As we mentioned, in the Mott insulator two of these auxiliary fermions describe the Hubbard bands. The third is pinned at the chemical potential, has no weight on the physical electron, and is crucial to enforce spin $SU(2)$ symmetry. Our evidence that such a Mott insulator has a paramagnetic response suggests that these hidden quasiparticles correspond to Anderson's spinons, neutral spin-1/2 excitations. Remarkably, these spinons reacquire spectral weight as soon as the Mott insulator is contacted with the metallic bath, giving rise to heavy-fermion quasiparticles, carrying both charge and spin, localized on a surface layer whose depth has the same critical behavior found within the conventional Gutzwiller wavefunction.

Our findings indicate that the zero-weight auxiliary fermions are firmly pinned at the chemical potential, regardless of its location within the Mott-Hubbard gap. Furthermore, they are prone to regaining spectral weight when in contact with a charge reservoir. Consequently, we anticipate that doping such a Mott insulator occurs without the chemical-potential jump expected from rigid Hubbard bands. Surface dopant adsorption on Ca_2RuO_4 provides a striking experimental confirmation of this scenario. Below $T_S = 357$ K, Ca_2RuO_4 is a paradigmatic Mott insulator, in which the compressive distortion of the RuO_6 octahedra drives the half-filled d_{xz}/d_{yz} sector across the Mott transition [50–52], see Fig. 3(b). Because bulk metallization routes, temperature, pressure, or chemical substitution, invariably proceed through the release of this structural distortion [50, 53, 54], carrier doping and chemical pressure cannot be disentangled in the bulk. Surface doping circumvents this obstruction: alkali-metal deposition was shown by angle-resolved photoemission to metallize the Mott-insulating surface through a single hybrid adatom Ru $4d$ in-gap band, leaving the short- c -axis structure, and hence the Mott background, intact [55]. Subsequent x-ray photoemission above the Néel transition revealed that electron (Cs) and hole (C_{60}) doping alike produce a low-binding-energy Ru $3d$ satellite, see Fig. 3(a), pinned at the chemical potential and without any gap-crossing jump, see Fig. 3(c). The coherent state thus develops within the Mott gap, on both sides of half filling, see Figs. 3(d),(e).

Taken together, these developments recast the Mott gap as a spectroscopically accessible arena: an ambipolar channel for metallization in which the in-gap states of the correlated insulator are converted into observable quasiparticles.

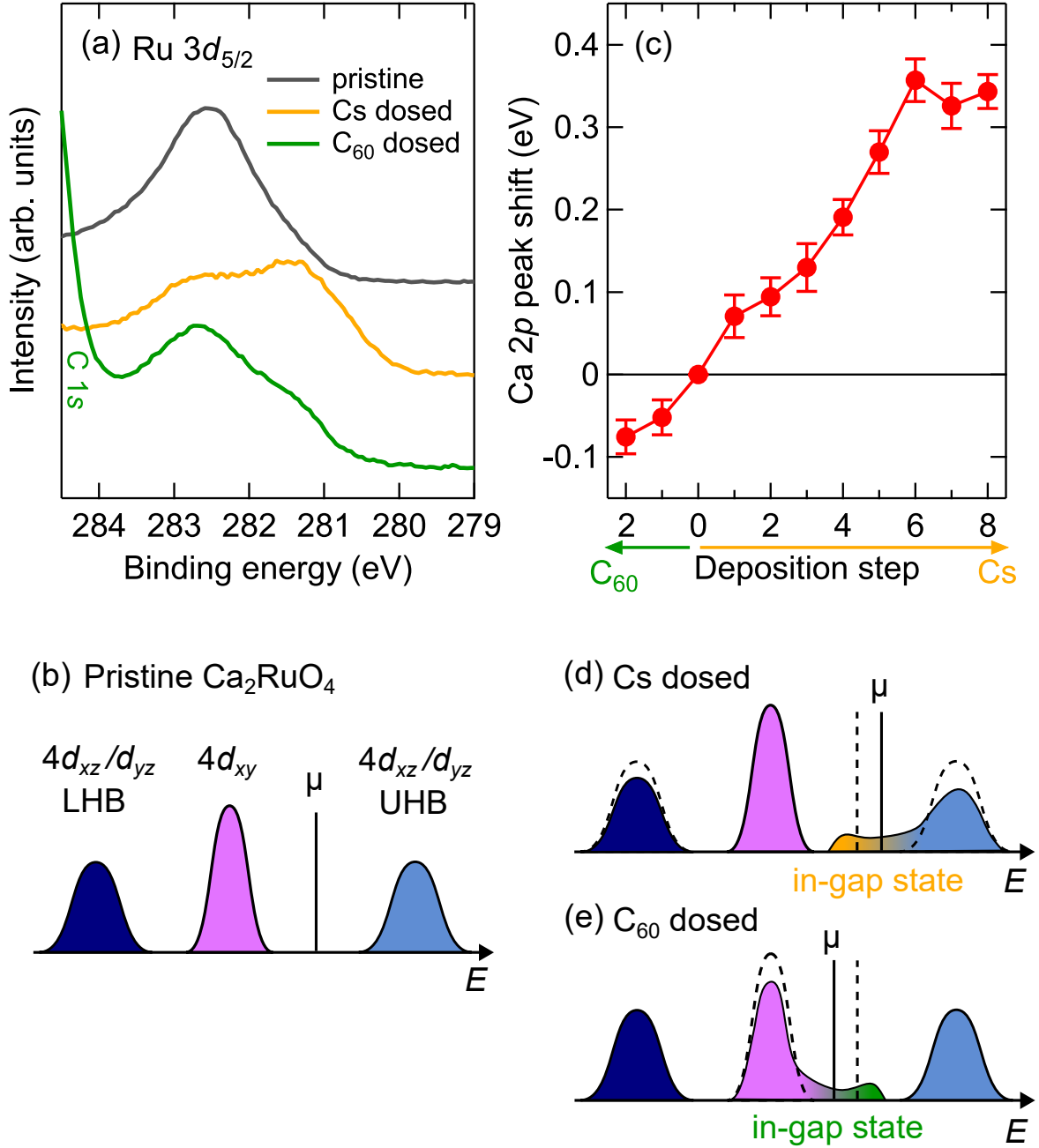


Figure 3: Ambipolar coherent in-gap state on surface-doped Ca_2RuO_4 . (a) Ru $3d$ core-level spectra of pristine, Cs-dosed (electron-doped), and C_{60} -dosed (hole-doped) Ca_2RuO_4 : both dopants generate a low-binding-energy satellite of comparable position (b) Level diagram of the pristine S-phase surface, with the filled $4d_{xy}$ band lying inside the d_{xz}/d_{yz} Mott gap. (c) Ca $2p$ core-level shift, (d),(e) Schematic in-gap state formation through hybridization between the dopant impurity level and the substrate for electron and hole doping, respectively. Adapted from Ref. [56].

1.2 Magnetism in Mott insulators

To further confirm the physical significance of the zero-weight auxiliary fermions that arise within the ghost-Gutzwiller approximation, we investigated in detail, within the ghost-Gutzwiller approach, the response of a symmetric single-band Mott insulator to both explicit and spontaneous $SU(2)$ symmetry breaking. We solve the variational problem by two different methods.

The number of variational parameters of the local operators in the ghost-Gutzwiller wavefunction is equal to the dimension of the product of the local physical and auxiliary Hilbert spaces. This number also corresponds to the number of wavefunction coefficients in an Anderson impurity model, where the impurity resides in the local physical Hilbert space and the baths in the local auxiliary Hilbert space. Consequently, the variational optimization of the local operators is equivalent to that of the impurity wavefunction, which can be directly achieved. Alternatively, one can introduce a set of Lagrange multipliers that, at the saddle point of the energy functional, should correspond to the components of the single-particle density matrix in the impurity wavefunction. In this manner, the variational problem is recast [9, 57] in terms of two self-consistently coupled eigenvalue problems: one for the impurity wavefunction and the other for the uncorrelated one. This problem can be readily solved iteratively.

Even though the direct optimization of the impurity wavefunction and the iterative scheme are intended to be equivalent, in reality they may not be, for two subtle reasons. In the iterative scheme, the use of the impurity single-particle density matrix as an unconstrained variational parameter faces the so called N -representability issue. As a result, there is no guarantee that the saddle point of the energy functional does correspond to the actual minimum. The second reason is even more subtle. The ghost-Gutzwiller wavefunction remains invariant under unphysical gauge transformations applied to the auxiliary fermions. In the metal, this gauge symmetry is completely broken. In contrast, in the Mott insulator, the gauge symmetry is fully restored for the zero-weight auxiliary fermions. Since this symmetry lacks a physical counterpart, it becomes challenging to enforce a gauge fixing, except when directly dealing with the impurity wavefunction. Consequently, in the iterative scheme, the solution to the impurity problem can oscillate between gauge-equivalent partners, hindering convergence. In a broader sense, this is the same difficulty encountered by DMFT in describing a spin-liquid insulator that we discussed earlier.

To elucidate this issue and the role of the zero-weight auxiliary fermions, we conducted a thorough analysis of the paramagnetic Mott insulator solutions obtained by the two alternative methods. By employing the direct optimization of the impurity wavefunction, we discovered that gauge fixing effectively eliminates most

of the gauge redundancy. However, a Z_2 gauge freedom remains, which is highly suggestive in relation to the spin-liquid phases achievable by the ghost-Gutzwiller approach. The optimization of the impurity wavefunction also suggests a way to force convergence in the iterative scheme, which we successfully confirm through a direct implementation.

The most significant distinction between the two methods becomes evident when we introduce a Zeeman splitting term that explicitly breaks the spin $SU(2)$ symmetry into $U(1)$. In this scenario, the direct optimization of the impurity wavefunction proves highly effective and provides compelling evidence that the Mott insulator exhibits a paramagnetic susceptibility, which aligns with the expectations for a spin-liquid insulator with a spinon Fermi surface. The crucial aspect of this solution is that the magnetization is carried solely by the zero-weight auxiliary fermions, the spinons, while the Hubbard bands remain unpolarized.

On the other hand, the iterative scheme can only converge to a fully polarized insulator, which is a legitimate state but has higher energy. Furthermore, the metal-Mott insulator transition in the presence of the Zeeman term is accompanied by a jump in the total energy, which is clearly unphysical. We suspect that the failure of the iterative scheme in this situation has to do with the aforementioned N -representability issue.

As we discussed, the primary challenge in describing a paramagnetic single-band Mott insulator using DMFT lies in the fact that DMFT is exact in infinite coordination lattices, where the true ground state is inevitably magnetically ordered. In fact, allowing for a spontaneous breaking of spin $SU(2)$ symmetry, DMFT is known to converge without any issue. Similarly, we find that the iterative scheme applied to the single-band Hubbard model, without enforcing $SU(2)$ symmetry, converges well to the expected antiferromagnetic insulator. In fact, the antiferromagnetic Mott insulator that we obtain within the ghost-Gutzwiller approach is very close to that obtained through the Hartree-Fock approximation, which is essentially a band insulator. Therefore, just as in the correlated metal phase, the gauge symmetry is found to be fully broken, thereby avoiding the issues discussed above. In this situation, the iterative scheme thus proves to be significantly more efficient than the impurity wavefunction optimization. Nevertheless, the latter method can be still employed, as we did, to tailor competitive variational states with tunable deviation from the simple Hartree-Fock antiferromagnetic insulator, quantified, e.g., by the local mutual information. These states, though metastable in infinite coordination lattices, should be more representative of antiferromagnetic insulators in finite coordination lattices where quantum fluctuations play a more significant role.

1.3 Plan of the Thesis

We here present the detailed plan of the Thesis.

In Chapter 2, we review the ghost-Gutzwiller wavefunction and approximation. We present the formalism for generic multiband models and introduce the impurity mapping. Furthermore, we present in detail the two different computational methods previously introduced, the direct optimization of the impurity wavefunction and the iterative scheme.

In Chapter 3 we present in more details the results outlined above in Sec. [1.1](#).

In Chapter 4 we instead discuss thoroughly the results here outlined in Sec. [1.2](#).

Chapter 5 is devoted to concluding remarks.

2 | THE GUTZWILLER AND GHOST GUTZWILLER APPROXIMATION

In this chapter, we introduce the ghost Gutzwiller wavefunction and the Gutzwiller approximation, which is derived from the conventional Gutzwiller wavefunction by introducing auxiliary fermionic degrees of freedom. These additional degrees of freedom enable the description of not only the low-energy quasiparticles captured in the conventional Gutzwiller wavefunction but also the high-energy Hubbard bands, which represent a significant improvement of the method. We formulate the method for a generic multi-band lattice model. After discussing how to compute expectation values in the Gutzwiller approximation, we delve into the relevant optimization methods for the variational parameters, specifically the variational method and the quantum embedding scheme.

In the Introduction 1, we discussed the necessity of a method capable of describing both the coherent quasiparticles and the high-energy spectral features of a Mott insulator on an equal footing. In this Chapter, we will formally construct such a method.

A powerful non perturbative approach in the study of strongly correlated systems is the Gutzwiller variational method, which relies on the Gutzwiller wavefunction [58]. Such wavefunction was originally introduced by Martin Gutzwiller to describe ferromagnetism in transition metals [59]. Concurrently, Gutzwiller proposed an approximate scheme to evaluate analytically the expectation values on his variational wavefunction, which is commonly known as the Gutzwiller approximation. Shortly afterwards, Brinkman and Rice [60] employed the Gutzwiller wavefunction and approximation to study the single-band half-filled Hubbard model, supposed to capture the physics of the prototype Mott insulator V_2O_3 . They were able to describe for the first time a Mott transition that, within the Gutzwiller approximation, occurs through a divergence of the effective mass, a behavior now known as the Brinkman-Rice scenario [60].

The Gutzwiller wavefunction is constructed by applying local linear operators $\mathcal{P}_i$ to a non-interacting Slater determinant or BCS wavefunction $|\psi_*\rangle$,

$$|\Psi\rangle = \prod_i \mathcal{P}_i |\psi_*\rangle . \quad (1)$$

In the original Gutzwiller wavefunction, the state $|\psi_*\rangle$ is defined on the Fock space of the original lattice. Consequently, the operator $\mathcal{P}_i$ acts on local configurations,

assigning them different weights compared to those in $|\psi_*\rangle$. The expectation values over (1) can be calculated analytically by the Gutzwiller approximation (GA), which has been shown to become exact in the limit of infinite dimension by Vollhardt and Metzner [5]. Despite its intuitive picture, Brinkman and Rice's description of the Mott transition fails to capture the high-energy Hubbard bands. Moreover, it offers a rather inadequate description of the Mott insulator as a collection of localized moments with an infinite magnetic susceptibility.

A recent extension of the standard Gutzwiller wavefunction and approximation [9], named *ghost* Gutzwiller wavefunction and approximation (ghost-GA), cures this problem. Within the ghost-GA approach, the Fock state $|\psi_*\rangle$ in (1) is defined in an enlarged Hilbert space built of N_{aux} auxiliary spinful fermions per site, as opposed to the $N_{phys} \leq N_{aux}$ physical electrons. The difference $N_{aux} - N_{phys} \geq 0$ is conventionally referred to as the number of ghosts N_{ghosts} . Consequently, the local operators $\mathcal{P}_i$ in Eq. (1) become linear maps from the enlarged local Hilbert space to the physical one. In the next paragraphs we will present in detail the method for a generic multi-band lattice model.

2.1 The ghost-Gutzwiller wavefunction for a multi-band lattice model

We consider a lattice model of N_{phys} electronic bands described by a tight-binding interacting Hamiltonian

$$H = \sum_{i \neq j} \mathbf{c}_i^\dagger \hat{t}_{ij} \mathbf{c}_j + \sum_i H_{loc}[\mathbf{c}_i^\dagger, \mathbf{c}_i], \quad (2)$$

where the matrix $\hat{t}_{ij}$ encodes the hopping amplitudes between different sites i and j , while H_{loc} collects the one- and two-body local terms. The $2N_{phys}$ -component spinors $\mathbf{c}_i$ denote the physical fermionic operators at site i , where the factor 2 comes from the spin. The auxiliary fermionic operators in the enlarged Hilbert space, instead, will be denoted by the $2N_{aux}$ -component spinors $\mathbf{f}_i$.

As remarked before, we can write the operator $\mathcal{P}_i$ as a linear map from the auxiliary Hilbert space to the physical one:

$$\mathcal{P}_i = \sum_{\Gamma_{phys} \gamma_{aux}} \Lambda_{\Gamma_{phys} \gamma_{aux}}(i) |\Gamma_{phys}, i\rangle \langle \gamma_{aux}, i|, \quad (3)$$

where $|\Gamma_{phys}, i\rangle$ and $|\gamma_{aux}, i\rangle$ denote the bases of the physical and auxiliary Hilbert spaces, respectively, at site i . In this section, we focus on the case with site-independent variational parameters $\Lambda_{\Gamma_{phys} \gamma_{aux}}$, the case of site-dependent variational

parameters will be considered in the next chapters when we deal with antiferromagnetic order. We note that the original Gutzwiller wavefunction is recovered for $N_{\text{aux}} = N_{\text{phys}}$.

The set of variational parameters defined by the matrix Λ with components $\Lambda_{\Gamma_{\text{phys}}\gamma_{\text{aux}}}$ and the state $|\psi_*\rangle$ is determined by minimizing the expectation value of the total energy:

$$E = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} . \quad (4)$$

Evaluating (4) is a complex task, and it generally requires numerical methods. However, the Gutzwiller approximation offers an analytical expression for the energy that is exact for lattices with infinite coordination and provides a seemingly good approximation even when the coordination is finite.

2.2 The Gutzwiller approximation and the Gutzwiller constraints

In order to evaluate the energy in equation (4), we introduce the following Gutzwiller constraints:

$$\begin{aligned} \langle \psi_* | \mathcal{P}_i^\dagger \mathcal{P}_i | \psi_* \rangle &= 1 , \\ \langle \psi_* | \mathcal{P}_i^\dagger \mathcal{P}_i \mathbf{f}_i \otimes \mathbf{f}_i^\dagger | \psi_* \rangle &= \langle \psi_* | \mathbf{f}_i \otimes \mathbf{f}_i^\dagger | \psi_* \rangle := \hat{\Delta}_*(\psi_*) . \end{aligned} \quad (5)$$

These constraints do not diminish the variational freedom. The first constraint is simply an overall normalization of Λ , which does not impact (4). The second constraint is essentially a *gauge-fixing*. Indeed, the wavefunction (1) remains invariant under the transformations $|\psi_*\rangle \rightarrow \prod_i U_i |\psi_*\rangle$ and $\mathcal{P}_i \rightarrow \mathcal{P}_i U_i^\dagger$, where U_i is a unitary gauge transformation $\in U(2N_{\text{aux}})$ whose generator are one-body operators. Therefore, the second constraint eliminates this unphysical gauge redundancy that does not affect (4).

Exploiting these constraints, the Gutzwiller approximation consists in neglecting all the expectation values that would vanish in the limit of infinite lattice-coordination number. Specifically, the approximation ignores all contributions to the expectation values over $|\psi_*\rangle$, which can be easily evaluated using Wick's theorem, involving more than two non-local Wick's contractions.

We note that, within the Gutzwiller approximation, the second constraint in (5) can be rewritten using Wick's theorem as:

$$\begin{aligned} \hat{\Delta}_*(\psi_*) &= \langle \psi_* | \mathcal{P}_i^\dagger \mathcal{P}_i \mathbf{f}_i \otimes \mathbf{f}_i^\dagger | \psi_* \rangle \\ &= \langle \psi_* | \mathcal{P}_i^\dagger \mathcal{P}_i | \psi_* \rangle \langle \psi_* | \mathbf{f}_i \otimes \mathbf{f}_i^\dagger | \psi_* \rangle + \overbrace{\langle \psi_* | \left(\mathcal{P}_i^\dagger \mathcal{P}_i \right) \left(\mathbf{f}_i \otimes \mathbf{f}_i^\dagger \right) | \psi_* \rangle} . \end{aligned}$$

It follows that,

$$\overline{\langle \psi_* | (\mathcal{P}_i^\dagger \mathcal{P}_i) (\mathbf{f}_i \otimes \mathbf{f}_i^\dagger) | \psi_* \rangle} = 0, \quad (6)$$

which implies that all the contractions involving the extraction of two fermionic lines from $\mathcal{P}_i^\dagger \mathcal{P}_i$ vanish.

This result greatly simplifies the analytic evaluation of the expectation values of local and non-local operators. Specifically,

- **Local Operators:** for a local operator $\mathcal{O}_i$, the GA implies that

$$\langle \Psi | \mathcal{O}_i | \Psi \rangle = \langle \psi_* | \mathcal{P}_i^\dagger \mathcal{O}_i \mathcal{P}_i | \psi_* \rangle. \quad (7)$$

- **Nonlocal Operators:** for an operator $\mathcal{O}_{ij}$ acting on different sites i and j , one finds that

$$\langle \Psi | \mathcal{O}_{ij} | \Psi \rangle = \langle \psi_* | \mathcal{P}_i^\dagger \mathcal{P}_j^\dagger \mathcal{O}_{ij} \mathcal{P}_i \mathcal{P}_j | \psi_* \rangle. \quad (8)$$

Let us apply the latter equation to the single-particle hopping:

$$\langle \Psi | \mathbf{c}_i \otimes \mathbf{c}_j^\dagger | \Psi \rangle = \langle \psi_* | \mathcal{P}_i^\dagger \mathcal{P}_j^\dagger \mathbf{c}_i \otimes \mathbf{c}_j^\dagger \mathcal{P}_i \mathcal{P}_j | \psi_* \rangle. \quad (9)$$

Due to the Gutzwiller approximation, the operators on sites i and j can only be contracted by a single fermionic line. This implies the following mapping valid inside the expectation value over a Slater determinant:

$$\mathcal{P}_i^\dagger \mathbf{c}_i \mathcal{P}_i \rightarrow \hat{R} \cdot \mathbf{f}_i, \quad (10)$$

where we introduced the wavefunction renormalization matrix $\hat{R}$ which is a $2N_{\text{phys}} \times 2N_{\text{aux}}$ matrix. Hence, the expectation value of the hopping term becomes

$$\langle \Psi | \mathbf{c}_i \otimes \mathbf{c}_j^\dagger | \Psi \rangle = \hat{R} \cdot \langle \psi_* | \mathbf{f}_i \otimes \mathbf{f}_j^\dagger | \psi_* \rangle \cdot \hat{R}^\dagger. \quad (11)$$

We note that the same wavefunction renormalization appears in the evaluation of the following expectation value:

$$\langle \psi_* | \mathcal{P}_i^\dagger \mathbf{c}_i \mathcal{P}_i \otimes \mathbf{f}_i^\dagger | \psi_* \rangle = \hat{R} \cdot \hat{\Delta}_*(\psi_*). \quad (12)$$

This equation enables the computation of the wavefunction renormalization matrix from quantities that are purely local.

In order to obtain more manageable expressions, it is useful to introduce the following matrix ϕ [61, 62]:

$$\phi_{\Gamma_{\text{phys}} \gamma_{\text{aux}}} = \left(\Lambda \cdot \sqrt{\rho_0} \right)_{\Gamma_{\text{phys}} \gamma_{\text{aux}}}, \quad (13)$$

where $(\rho_0)_{\gamma\gamma'} = \langle \psi_* | \gamma', i \rangle \langle \gamma, i | \psi_* \rangle$ is the local density matrix of the auxiliary fermions, while γ and γ' are local configurations of the auxiliary Fock space. In terms of the ϕ matrix, the Gutzwiller constraints can be rewritten as:

$$\begin{aligned} \text{Tr}(\phi^\dagger \phi) &= 1, \\ \langle \psi_* | \mathbf{f}_i \otimes \mathbf{f}_i^\dagger | \psi_* \rangle &= \text{Tr}(\phi^\dagger \phi \mathbf{f} \otimes \mathbf{f}^\dagger) = \hat{\mathbb{I}} - \hat{\Delta}_\phi, \end{aligned} \quad (14)$$

where in the second equation, we omitted the site label i since the ϕ matrix does not depend on the spatial index. By $\mathbf{f} \otimes \mathbf{f}^\dagger$ we mean its matrix representation on the local basis where ϕ is defined. Notably, since ρ_0 is the local reduced density matrix of a Slater determinant, it has a closed expression in terms of the $\hat{\Delta}_\phi$ matrix [63], namely:

$$(\rho_0)_{\gamma\gamma'} = \left[\exp(-i \mathbf{f}^\dagger \hat{\xi} \mathbf{f}) \right]_{\gamma\gamma'}, \quad (15)$$

where

$$\hat{\xi} = \ln \frac{\hat{\mathbb{I}} - \hat{\Delta}_\phi}{\hat{\Delta}_\phi}.$$

In terms of the ϕ matrix, the equation for the wavefunction renormalization matrix in (12) can be rewritten as:

$$\hat{R}(\phi) \cdot \hat{\Delta}_\phi = \text{Tr} \left(\phi^\dagger \mathbf{c} \phi \otimes \sqrt{\rho_0^{-1}} \mathbf{f}^\dagger \sqrt{\rho_0} \right). \quad (16)$$

Through the identity

$$\rho_0^\dagger \mathbf{f}^\dagger \rho_0 \equiv \mathbf{e}^{i \hat{\xi}} \cdot \mathbf{f}^\dagger, \quad (17)$$

we can write the equation for the wavefunction renormalization matrix as:

$$\hat{R}(\phi) \cdot \hat{S}(\hat{\Delta}_\phi) = \text{Tr}(\phi^\dagger \mathbf{c} \phi \mathbf{f}^\dagger), \quad (18)$$

where

$$\hat{S}(\hat{\Delta}_\phi) = \sqrt{\hat{\Delta}_\phi (\hat{\mathbb{I}} - \hat{\Delta}_\phi)}. \quad (19)$$

Combining all the previous expressions, we get a final expression for the variational energy in the Gutzwiller approximation:

$$\mathcal{E} = \langle \psi_* | \mathcal{H}_* | \psi_* \rangle + \sum_i \text{Tr}(\phi^\dagger \mathcal{H}_{\text{loc},i} \phi), \quad (20)$$

where

$$\mathcal{H}_* = \sum_{i \neq j} \mathbf{f}_i^\dagger \hat{R}(\phi)^\dagger \hat{t}_{ij} \hat{R}(\phi) \mathbf{f}_j. \quad (21)$$

2.3 Mapping onto an impurity state

In this section, we rewrite the traces over the ϕ matrix as expectation values over an impurity state. This is a useful step to connect the Gutzwiller and ghost-Gutzwiller approximations to a class of methods known as quantum embedding methods [64]. We note that the matrix ϕ has the same number of entries as an impurity wavefunction defined in a Hilbert space of N_{aux} bath spinful fermions and N_{phys} impurity spinful fermions. Specifically, we can define the impurity state as:

$$|\phi\rangle = \sum_{\Gamma_{phys}\gamma_{aux}} \phi_{\Gamma_{phys}\gamma_{aux}} e^{iN_{\gamma_{aux}}(N_{\gamma_{aux}}-1)/2} \mathcal{U}_{ph} |\gamma_{aux}\rangle |\Gamma_{phys}\rangle, \quad (22)$$

where N_{γ} is the total number of fermions in the state $|\gamma\rangle$, and $\mathcal{U}_{ph}$ is a properly defined particle-hole transformation that acts only on the auxiliary fermion Hilbert space. In terms of the impurity wavefunction, the Gutzwiller constraints can be rewritten as:

$$\langle\phi|\phi\rangle = 1, \quad \hat{\Delta}_*(\psi_*) = \hat{\mathbb{I}} - \langle\phi|\mathbf{f} \otimes \mathbf{f}^\dagger|\phi\rangle = \hat{\mathbb{I}} - \hat{\Delta}_\phi. \quad (23)$$

Furthermore, given any physical local operator $\mathcal{O}$, one can demonstrate within the ghost-Gutzwiller approximation the following equivalence

$$\langle\Psi|\mathcal{O}[\mathbf{c}_i^\dagger, \mathbf{c}_i]|\Psi\rangle \equiv \langle\phi|\mathcal{O}[\mathbf{c}^\dagger, \mathbf{c}]|\phi\rangle. \quad (24)$$

In terms of the impurity state, the equation defining the wavefunction renormalization can be written as:

$$\hat{R}(\phi) \cdot S(\hat{\Delta}_\phi) = \hat{Q}(\phi), \quad (25)$$

with

$$\hat{Q}(\phi) = \langle\phi|\mathbf{c} \otimes \mathbf{f}^\dagger|\phi\rangle. \quad (26)$$

Finally, the expression for the energy functional per site that we need to minimize becomes:

$$\mathcal{E}(\psi_*, \phi) = \frac{1}{V} \sum_{i \neq j} \langle\psi_*|\mathbf{f}_i^\dagger \hat{R}(\phi)^\dagger \hat{t}_{ij} \hat{R}(\phi) \mathbf{f}_j|\psi_*\rangle + \langle\phi|\mathcal{H}_{loc}[\mathbf{c}^\dagger, \mathbf{c}]|\phi\rangle, \quad (27)$$

with V the number of sites. Equivalently, enforcing the constraints (23) through a Lagrange multiplier matrix $\hat{\lambda}$, and the normalizations of $|\psi_*\rangle$ and $|\phi\rangle$ by two additional Lagrange multipliers E_* and E_ϕ , respectively, the minimization of (27) translates to finding the saddle point of the functional

$$\mathcal{F} = \mathcal{E}(\psi_*, \phi) - E_* \langle\psi_*|\psi_*\rangle - E_\phi \langle\phi|\phi\rangle + \text{Tr} \left(\hat{\lambda} \cdot \left\{ \hat{\mathbb{I}} - \hat{\Delta}_\phi - \hat{\Delta}_*(\psi_*) \right\} \right). \quad (28)$$

The saddle-point equation for $|\psi_*\rangle$ is just the ground-state problem of a non-interacting Hamiltonian whose parameters depend on $|\phi\rangle$ and $\hat{\lambda}$. The equation for $|\phi\rangle$, by contrast, is a non-linear Schrödinger equation, since the functional

derivative of $\hat{R}(\phi)$ in (12) is not linear in $|\phi\rangle$. Even so, one can always adopt a suitable parametrization of $|\phi\rangle$ and search directly for the saddle point of (28) without ever solving the non-linear Schrödinger equation; we will refer to this as the *variational method*. We will explore this method in Chapter 4, where we will highlight how this method can capture magnetic properties of Mott insulators at zero temperature and how other methods can fail despite being more computationally efficient.

2.3.1 Minimization via the embedding scheme

An alternative route to the stationary point of the functional (28) is the *iterative embedding scheme*, in which additional Lagrange multipliers turn the equation for the impurity wavefunction into a linear eigenvalue problem, so that $|\phi\rangle$ becomes the ground state of an impurity model. Specifically, one introduces the Lagrange multiplier matrix $\hat{V}$ to enforce equation (25), while treating $\hat{R}$ as an independent parameter. Furthermore, a variational density matrix $\hat{\Delta}$ is introduced, together with the Lagrange multiplier matrices $\hat{\lambda}$ and $\hat{\lambda}^c$ that force $\hat{\Delta}_*(\psi_*)$ and $\hat{\Delta}_\phi$ to be equal to $\hat{\Delta}$. The functional to be extremized then becomes

$$\begin{aligned} \mathcal{L} = & \mathcal{E}'(\psi_*, \hat{R}) - E_* \langle \psi_* | \psi_* \rangle - E_\phi \langle \phi | \phi \rangle \\ & + \text{Tr} \left(\hat{\lambda} \cdot \left(\hat{\Delta}_*(\psi_*) - \hat{\Delta} \right) \right) - \text{Tr} \left(\hat{\lambda}^c \cdot \left(\mathbb{I} - \hat{\Delta}_\phi - \hat{\Delta} \right) \right) \\ & + \text{Tr} \left(\left(\hat{R} \cdot \hat{S}(\hat{\Delta}) - \hat{Q}(\phi) \right) \cdot \hat{V} + H.c. \right), \end{aligned} \quad (29)$$

where $\mathcal{E}'(\psi_*, \hat{R})$ is derived from $\mathcal{E}(\psi_*, \phi)$ in (27) replacing $\hat{R}(\phi)$ with $\hat{R}$, while $\hat{S}(\hat{\Delta})$ is obtained from the equation 19 replacing $\hat{\Delta}_\phi$ with $\hat{\Delta}$. After these manipulations, the saddle-point equations of (29) can be cast as a set of self-consistency conditions that bear a very close resemblance to the DMFT self-consistency loop [13], the significant difference being that they require only the ground state of the impurity model rather than its frequency-dependent Green's function. As in DMFT, this saddle point is

then readily reached through iterative methods.

In particular, the equations for the embedding scheme to be solved iteratively are:

$$\begin{aligned}
\mathcal{H}_{qp}(\hat{R}, \hat{\lambda}) |\psi_*\rangle &= E_* |\psi_*\rangle , \\
\mathcal{H}_{imp}(\hat{V}, \hat{\lambda}_c) |\phi\rangle &= E_\phi |\phi\rangle , \\
\hat{R} \cdot \hat{S}(\hat{\Delta}) &= \hat{Q}(\phi) , \\
\hat{V} \cdot \hat{S}(\hat{\Delta}) &= \frac{1}{V} \sum_{i \neq j} \langle \psi_* | \mathbf{f}_i^\dagger \hat{R}^\dagger \hat{t}_{ij} \mathbf{f}_j | \psi_* \rangle , \\
\hat{\Delta} &= \hat{\Delta}_*(\psi_*), \\
\hat{\Delta} &= \mathbb{I} - \hat{\Delta}_\phi , \\
\hat{\lambda}^c &= -\hat{\lambda} + \frac{\delta}{\delta \hat{\Delta}} \text{Tr} \left(\left(\hat{R} \cdot \hat{S}(\hat{\Delta}) - \hat{Q}(\phi) \right) \cdot \hat{V} + H.c. \right) ,
\end{aligned} \tag{30}$$

where we introduce the impurity and quasiparticle Hamiltonians:

$$\begin{aligned}
\mathcal{H}_{qp}(\hat{R}, \hat{\lambda}) &= \sum_{ij} \mathbf{f}_i^\dagger \hat{R}^\dagger \hat{t}_{ij} \hat{R} \mathbf{f}_j - \sum_i \mathbf{f}_i^\dagger \hat{\lambda} \mathbf{f}_i , \\
\mathcal{H}_{imp}(\hat{V}, \hat{\lambda}_c) &= \mathcal{H}_{loc}[\mathbf{c}^\dagger, \mathbf{c}] + \mathbf{f} \hat{\lambda}^c \mathbf{f}^\dagger + \left(\mathbf{f}^\dagger \hat{V} \mathbf{c} + H.c. \right) .
\end{aligned} \tag{31}$$

It should be stressed, however, that promoting the one-body density matrices $\hat{\Delta}$ and $\hat{R}$ in (29) to free variational parameters is a non-trivial assumption, since these objects obey strong representability constraints [65]. As a consequence, the minimum of the variational energy (27) may lie on the boundary of the region where the one-body density matrices are defined, rather than at a saddle point of (29). As we shall see, this is precisely what happens in the Mott insulating phase, where some entries of $\hat{R}$ vanish and the minimum is pushed to the boundary of the admissible region—a regime in which the embedding scheme becomes especially delicate.

2.4 Spectral properties within the ghost-Gutzwiller approximation

In this section, we investigate the approximate spectral properties of a lattice Hamiltonian in the ghost-Gutzwiller approximation. In particular, we consider the matrix spectral function built from the physical spinor $\mathbf{c}_\mathbf{k}$:

$$\hat{\mathcal{A}}_\mathbf{k}(\omega) = \langle \psi | \mathbf{c}_\mathbf{k} \delta(\omega + \hat{\mathcal{H}}) \otimes \mathbf{c}_\mathbf{k}^\dagger | \psi \rangle + \langle \psi | \mathbf{c}_\mathbf{k}^\dagger \delta(\omega - \hat{\mathcal{H}}) \otimes \mathbf{c}_\mathbf{k} | \psi \rangle , \tag{32}$$

with $\mathbf{c}_{\mathbf{k}} = \frac{1}{\sqrt{V}} \sum_i e^{-i\mathbf{k}\mathbf{R}_i} \mathbf{c}_i$. The entries of (32) reproduce the index-resolved spectral function. To evaluate the matrix spectral function, it is useful to introduce the following quantities:

$$\begin{aligned}\hat{\mathcal{H}}_{qp}(\mathbf{k}) &= \mathbf{f}_{\mathbf{k}}^\dagger \hat{t}_{\mathbf{k}}^{qp} \mathbf{f}_{\mathbf{k}} , \\ \hat{t}_{\mathbf{k}}^{qp} &= \sum_{i,j} e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} \left(\hat{R}^\dagger \hat{t}_{ij} \hat{R} - \hat{\lambda} \delta_{ij} \right) , \\ \mathbf{f}_{\mathbf{k}} &= \frac{1}{\sqrt{V}} \sum_i e^{-i\mathbf{k}\mathbf{R}_i} \mathbf{f}_i .\end{aligned}\tag{33}$$

We now insert an approximate set of states corresponding to the so-called Landau-Gutzwiller quasi-particles [66],

$$\left| \psi_{G,\mathbf{k}}^p \right\rangle = \prod_i \mathcal{P}_i \mathbf{h}_{\mathbf{k}}^\dagger |\psi_*\rangle , \quad \left| \psi_{G,\mathbf{k}}^h \right\rangle = \prod_i \mathcal{P}_i \mathbf{h}_{\mathbf{k}} |\psi_*\rangle ,\tag{34}$$

where $\mathbf{h}_{\mathbf{k}}$ denotes the spinor of eigenoperators of the quasiparticle Hamiltonian matrix $\hat{\mathcal{H}}_{qp}(\mathbf{k})$ defined from (33). Inserting these approximate many-body excitations in the expression for the spectral function, we obtain the compact matrix expression (see the Appendix of [9] for a detailed derivation):

$$\hat{\mathcal{A}}_{\mathbf{k}}(\omega) = \hat{R}^\dagger \delta(\omega - \hat{t}_{\mathbf{k}}^{qp}) \hat{R} ,\tag{35}$$

Furthermore, through the Hilbert transform we can obtain the following expression for the single-particle Green's function:

$$\hat{\mathcal{G}}_{\mathbf{k}}(\omega) = \hat{R}^\dagger \frac{1}{\omega - \hat{t}_{\mathbf{k}}^{qp}} \hat{R} ,\tag{36}$$

Remarkably, one can also obtain a closed expression for the self-energy starting from the previous expression [67]:

$$\Sigma(z) = z - \left(\hat{R}^\dagger \cdot (z - \hat{\lambda})^{-1} \cdot \hat{R} \right)^{-1} .\tag{37}$$

2.5 Conclusions

In this Chapter we have introduced the ghost-Gutzwiller wavefunction and approximation for a generic multi-band lattice model, formulated the variational energy functional, and shown how it can be recast either as a direct optimization over an impurity wavefunction or as a set of self-consistent equations reminiscent of DMFT. We also derived the corresponding expressions for the spectral function, the Green's function, and the self-energy. Equipped with this formalism, in Chapter 3 we apply it to the interface between a Mott insulator and a metal, while in Chapter 4 we compare the direct variational and embedding minimization schemes in detail, in the context of magnetism in Mott insulators.

3

REVEALING SPINONS BY
PROXIMITY EFFECT

The ghost-Gutzwiller variational wavefunction within the Gutzwiller approximation, introduced in Chapter 2, is shown to stabilise a genuine paramagnetic Mott insulator in the half-filled single-band Hubbard model. This phase hosts quasiparticles that are crucial to the paramagnetic response without showing up in the single-particle spectrum, and, as such, they can be legitimately regarded as an example of Anderson’s spinons. We demonstrate that these spinons at the interface with a metal reacquire charge by proximity effect and thus reemerge in the spectrum as a heavy-fermion band. This heavy-fermion proximity effect offers a simple explanation of recent experiments in surface-doped systems.

In this Chapter we discuss the first application of the ghost-GA previously introduced, namely the study of an interface between a metal and a paramagnetic Mott insulator. To describe the physics of the system we will highlight the role of neutral quasiparticles, which are the hallmark of quantum spin liquids.

Quantum spin liquids are Mott insulators that host local moments which do not order down to very low temperatures and yet exhibit mutual long-range quantum entanglement well above those temperatures [7, 8]. The elementary excitations of such systems at energies below the Mott-Hubbard single-particle gap cannot carry electric charge, but they may carry spin as well as possibly emergent quantum numbers [7, 8, 68–70]. A celebrated example of these excitations are Anderson’s spinons [71, 72], which arise in the uniform resonating valence bond states proposed to describe highly frustrated spin-1/2 Heisenberg models and weakly-doped Mott insulators [71–74]. These are neutral gapless spin-1/2 quasiparticles that possess a well-defined *Fermi surface*. Even though such Fermi surface is likely to suffer from a low-temperature instability opening a finite spin-gap Δ_{sp} [75–79], one could envisage the possibility of a spinon degeneracy temperature T_{sp} much larger than Δ_{sp} , which would imply that gapless spinons still characterize the physical behavior for temperatures $\Delta_{sp} \ll T \ll T_{sp}$, or, possibly, at finite magnetic fields [80]. In those circumstances, a spinon Fermi surface would reveal itself in inelastic neutron scattering [81, 82] or thermal properties [83–88]. Alternatively, spinons can be detected by more local probes, e.g., through their ability to Kondo screen magnetic impurities [89–91], or by making proper interfaces with the quantum spin-liquid [32, 33, 92–94].

In this Chapter, we show that even the simplest interface with a conventional metal might be suitable to reveal the spinons hosted in a quantum spin-liquid

Mott insulator. Hereafter, we assume a simplified portrait of a quantum spin-liquid, specifically, the paramagnetic Mott insulator that can be stabilized in the single-band Hubbard model forcing spin- $SU(2)$ symmetry within ghost-GA [9]. Such interface, as already mentioned in the Introduction 1, has already been studied at particle-hole symmetry by Helmes, Costi and Rosch [95] using dynamical mean-field theory (DMFT) [96]. They showed that the metal penetrates inside the Mott insulator creating a narrow quasiparticle peak that decays exponentially inside the insulating slab over a length that corresponds to the correlation length associated to the Mott transition. This result, later reproduced in [97] using the standard Gutzwiller approximation, was interpreted as a Kondo-like proximity effect: the Mott insulator hosts localized moments which are promoted into genuine Kondo resonances by the coupling with the metal [95]. While it seems tempting to identify those local moments with spinons *a priori*, such an interpretation does not stand up to detailed scrutiny. Indeed, the paramagnetic Mott insulator that is stabilized in DMFT has an extensive spin entropy, $\ln 2$ per site [96], as if the local moments were completely free, thus lacking the massive entanglement characterizing quantum spin liquids. Exactly the same occurs in the standard Gutzwiller approximation [60], where the Mott insulator is a trivial state of independent sites, each occupied by a single electron. In the meantime, the DMFT Mott insulator is claimed to exhibit a finite uniform paramagnetic spin susceptibility [96], which seems not truly consistent with its extensive entropy, nor with the evidence that a straight $T = 0$ DMFT calculation in the Mott insulator at weak magnetic fields does not converge or finds a fully polarized solution [98], barring access to the magnetic susceptibility calculated through the magnetization versus field. We will show in Chapter 4 that the inability to faithfully describe a Mott insulator in a magnetic field is a general problem of quantum embedding schemes when implemented iteratively.

To address this shortcoming, we decided to use the *ghost*-Gutzwiller approximation [9] discussed in Chapter 2 which is able to stabilize a genuine, zero-entropy, paramagnetic Mott insulator [99]. This hints at the existence of spinons, whose presence we aim to trace out. In particular, and to better highlight the chargeless nature of spinons, in this Chapter we investigate a metal-Mott insulator interface away from the particle-hole (p-h) symmetric value of the chemical potential. For completeness, we start with the standard Gutzwiller approximation [58, 59, 61, 100–102], since the Mott transition changes nature away from p-h symmetry and becomes first order. This change of character has been exploited in [103] to study by DMFT the interface between metal and Mott insulator phases coexisting at equilibrium. We next move to the main part of our work, namely, the interface studied by the *ghost*-Gutzwiller approximation [9, 99, 104–111].

Specifically, the Chapter is organised as follows: in section (3.1) we give a brief introduction to the model for the Metal-Mott interface and we will discuss the implementation of the GA and the ghost-GA in this particular setting. In section

(3.2), we present results using the standard GA and show how the phenomenology of the Kondo proximity effect extends to non particle-hole symmetric cases. In section 3.3 we study the same model by the ghost-GA. Finally, in section 3.4, we discuss the results by solving analytically the ghost-GA variational problem for a bulk Mott insulator in the limit of a very large Mott-Hubbard gap. In that limit, we also show the solution forcing a finite spin-polarization, which clearly unveils the role of spinon in allowing the Mott insulator to sustain partial spin-polarization, and gives access to the paramagnetic susceptibility. Section 3.5 is devoted to conclusions and outlooks.

3.1 Model and methods

In Fig. 4 we show the system under investigation, which consists of a set of metallic layers, represented as weakly interacting Hubbard models, coupled to several Mott insulating ones, strongly interacting Hubbard models. The system has a total of N layers and the interlayer coupling is just a single particle hopping. We assume that intralayer and interlayer hopping strengths are equal, while the difference between metallic and Mott-insulating layers is modelled by a layer-dependent Hubbard repulsion. The system is therefore described by the Hamiltonian:

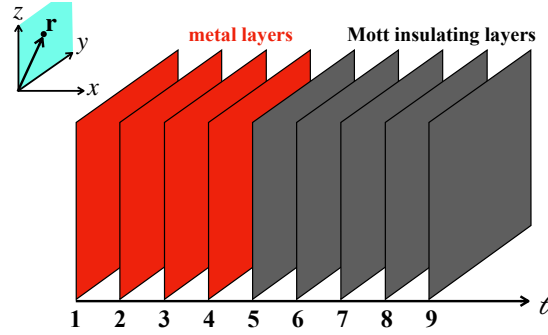


Figure 4: Schematic representation of the slab geometry in the case of 9 layers, 4 of which are metallic, in red, and the rest Mott insulating, in grey. Layers are stacked along the x -axis, while a site in each layer is identified by the vector $\mathbf{r}$ in the y - z plane.

$$\begin{aligned} \mathcal{H} = & \sum_{\ell=1}^N \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\ell\mathbf{k}\sigma}^\dagger c_{\ell\mathbf{k}\sigma} - t \sum_{\ell=1}^{N-1} \sum_{\mathbf{k}\sigma} (c_{\ell+1\mathbf{k}\sigma}^\dagger c_{\ell\mathbf{k}\sigma} + H.c.) \\ & + \sum_{\ell=1}^N \sum_{\mathbf{r}} \left\{ \frac{U_\ell}{2} (n_{\ell\mathbf{r}} - 1)^2 - \delta\mu n_{\ell\mathbf{r}} \right\}, \end{aligned} \quad (38)$$

where the lattice sites are identified by an intralayer coordinate $\mathbf{r}$ and a layer index $\ell = 1, \dots, N$, and thus $n_{\ell\mathbf{r}}$ is the on-site occupation number, the non-interacting intra-layer dispersion is $\epsilon_{\mathbf{k}} = -2t (\cos k_y + \cos k_z)$, with $\mathbf{k}$ the momentum in the y - z

plane, and σ labels the spin of the electrons. Hereafter, we take $t = 1$ as energy unit. We remark that $\delta\mu$ in Eq. (38) parametrizes the deviation of each layer with respect to the p-h symmetric case, $\delta\mu = 0$, while the physical layer-dependent *chemical* potential is in reality $\mu_\ell = U_\ell/2 + \delta\mu$.

We now discuss the details of the Gutzwiller (both standard and ghost) approximation for the system under investigation. For the case of the Hamiltonian in Eq. (38) the variational wavefunction 1 reads:

$$|\Psi\rangle = \mathcal{P}_G |\Psi_*\rangle, \quad \mathcal{P}_G = \prod_{\mathbf{r}, \ell} \left\{ \sum_{\gamma, \Gamma} \Lambda_{\Gamma, \gamma}(\ell) |\mathbf{r}, \ell; \Gamma\rangle \langle \mathbf{r}, \ell; \gamma| \right\}, \quad (39)$$

where we remark that the states γ are local Fock states of the auxiliary fermions, whose annihilation operators we denote as $d_{\ell\mathbf{r}\alpha\sigma}$, $\alpha = 1, \dots, N_{aux}$ spanning the auxiliary spinful orbitals. On the contrary, the set Γ includes the local physical Fock states.

In Eq. (39) we have assumed translational invariance within each layer, so that our variational parameters depend only on the ℓ coordinate. This also implies that the variational wavefunction Eq. (39) cannot develop the antiferromagnetic order parameter that characterizes the actual ground state of Eq. (38) at finite on-site repulsion. Such a restriction into a subspace of the whole Hilbert space, which does not include the expected ground state in the specific example, is easy to implement in the variational approach.

As outlined in Chapter 2, following [102] we can associate the parameters $\Lambda_{\Gamma, \gamma}(\mathbf{r}, \ell)$ to the components of a wavefunction that describes an impurity coupled to N_{aux} baths. In the slab geometry, we need an impurity wavefunction $|\phi(\ell)\rangle$ for each layer. Using the Gutzwiller approximation, specified in the paragraph (2.2), we can write the variational energy as:

$$E[\Psi] = \langle \Psi_* | \mathcal{H}_* | \Psi_* \rangle + \mathcal{A} \sum_{\ell} \langle \phi(\ell) | \mathcal{H}_{loc}(\ell) | \phi(\ell) \rangle, \quad (40)$$

with $\mathcal{A}$ the number of sites within each layer,

$$\mathcal{H}_* = \sum_{\mathbf{k}\ell\ell'\sigma} \sum_{\alpha\beta} d_{\ell\mathbf{k}\alpha\sigma}^\dagger R_{\alpha\sigma}^\dagger(\ell) t_{\ell\ell'}(\mathbf{k}) R_{\beta\sigma}(\ell') d_{\ell'\mathbf{k}\beta\sigma}, \quad (41)$$

where $t_{\ell\ell'}(\mathbf{k}) = \epsilon(\mathbf{k}) \delta_{\ell\ell'} - t \sum_{p=\pm 1} \delta_{\ell', \ell+p}$, and

$$\mathcal{H}_{loc}(\ell) = \frac{U_\ell}{2} (n_\ell - 1)^2 - \delta\mu n_\ell, \quad (42)$$

with n_ℓ the occupation number of the impurity level. As mentioned in equation (10), the vector $\mathbf{R}(\ell)$ with components $R_{\alpha\sigma}(\ell)$ in Eq. (41), defined in Eq. (A.2) of the Appendix A.1 for this specific model, looks like a wavefunction renormalization,

$$c_{\ell\mathbf{k}\sigma} \rightarrow \sum_{\alpha} R_{\alpha\sigma}(\ell) d_{\ell\mathbf{k}\alpha\sigma},$$

suggesting that $d_{\ell\mathbf{k}\alpha\sigma}$ can be identified with the quasiparticle Fermi operators.

In this Chapter we will use the iterative embedding scheme, presented in section 2.3.1, to minimize the energy in Eq. (40). In particular, the quasiparticle Hamiltonian $\mathcal{H}^{qp}$, and the impurity Hamiltonians $\mathcal{H}_{imp}(\ell)$ for each layer, as reported in equation (31), read:

$$\mathcal{H}^{qp} = \mathcal{H}_* - \sum_{\mathbf{k}\ell\sigma} \sum_{\alpha\beta} d_{\ell\mathbf{k}\alpha\sigma}^\dagger \lambda_{\alpha\sigma,\beta\sigma}(\ell) d_{\ell\mathbf{k}\beta\sigma} = \sum_{\mathbf{k}\sigma} \mathcal{H}_{\mathbf{k}\sigma}^{qp}, \quad (43)$$

and

$$\mathcal{H}_{imp}(\ell) = \mathcal{H}_{loc}(\ell) + \sum_{\alpha\sigma} V_{\alpha\sigma} (d_{\ell\alpha\sigma}^\dagger c_{\ell\sigma} + H.c.) - \sum_{\alpha\beta\sigma} d_{\ell\alpha\sigma}^\dagger \lambda_{\alpha\sigma,\beta\sigma}^c(\ell) d_{\ell\beta\sigma}. \quad (44)$$

The self-consistency condition is expressed in terms of the one-body reduced density matrices of the impurity model and of the quasi-particle Hamiltonian:

$$\langle \phi(\ell) | d_{\ell\alpha\sigma} d_{\ell\beta\sigma}^\dagger | \phi(\ell) \rangle = \langle \Psi_* | d_{\ell\mathbf{r}\beta\sigma}^\dagger d_{\ell\mathbf{r}\alpha\sigma} | \Psi_* \rangle. \quad (45)$$

As explained in section 2.3.1, the Hamiltonians Eq. (43) and Eq. (44) depend on a set of Lagrange multipliers $\lambda_{\alpha\sigma,\beta\sigma}^c(\ell)$, $\lambda_{\alpha\sigma,\beta\sigma}(\ell)$ and $V_{\alpha\sigma}(\ell)$. We report the iterative embedding equation for this model in Appendix A.1. The parameter $V_{\alpha\sigma}(\ell)$ is the hybridisation between the impurity and the baths, while $\lambda_{\alpha\sigma,\beta\sigma}^c(\ell)$ and $\lambda_{\alpha\sigma,\beta\sigma}(\ell)$ are one-body potentials for the bath levels and the quasiparticles, respectively. It is worth emphasizing that the physical chemical potential $\mu = U/2 + \delta\mu$ translates into the energy level of the impurity, see Eq. (42). Through the energy minimization and the self-consistency equation (45), μ plays a role in determining the local potential $\lambda_{\alpha\sigma,\beta\sigma}(\ell)$ of the quasiparticle Hamiltonian in Eq. (41), and thus the position of the quasiparticle bands.

Through the knowledge of the quasiparticle Hamiltonian, we can obtain the approximate expression for the Green's function matrix 36 for each layer which allows defining an approximate self-energy $\Sigma(\omega, \ell, \mathbf{k})$ and a layer-dependent quasiparticle residue:

$$Z(\ell, \mathbf{k}) = \left(1 - \frac{\partial \Sigma(\omega, \ell, \mathbf{k})}{\partial \omega} \Big|_{\omega=0} \right)^{-1}. \quad (46)$$

Other local observables can be obtained through the impurity wavefunction. In particular, we will be interested in the electron density per layer given by:

$$n_\ell = \sum_{\sigma} \langle \phi(\ell) | c_{\ell\sigma}^\dagger c_{\ell\sigma} | \phi(\ell) \rangle.$$

3.2 Wetting critical behavior in the standard Gutzwiller approximation

Using the variational ansatz in Eq. (39) with $N_{aux} = 1$, thus the standard Gutzwiller wavefunction, we can study the fate of the Kondo-like proximity effect

away from p-h symmetry. In the standard GA, just as in DMFT, the Mott transition away from particle-hole symmetry becomes genuinely first-order. In other words, there is a range of $U \in [U_{c1}, U_{c2}]$, bounded by the insulator and metal spinodal points, U_{c1} and $U_{c2} > U_{c1}$, respectively, where the two phases coexist. Their corresponding energies cross at U_c in between the spinodal values. At particle-hole symmetry, U_c accidentally coincides with U_{c2} in DMFT, while, in standard GA, the transition turns second order.

One may wonder how such change of character in the transition affects the proximity effect observed in [95, 97]. It is known that approaching a first-order phase transition one can still find a surface critical phenomenon, the wetting transition [112]. It was conjectured in [113], using an effective spin model for the Mott transition, that the Kondo proximity effect becomes an example of total wetting [114] when the Mott transition is discontinuous. We quantitatively address this question

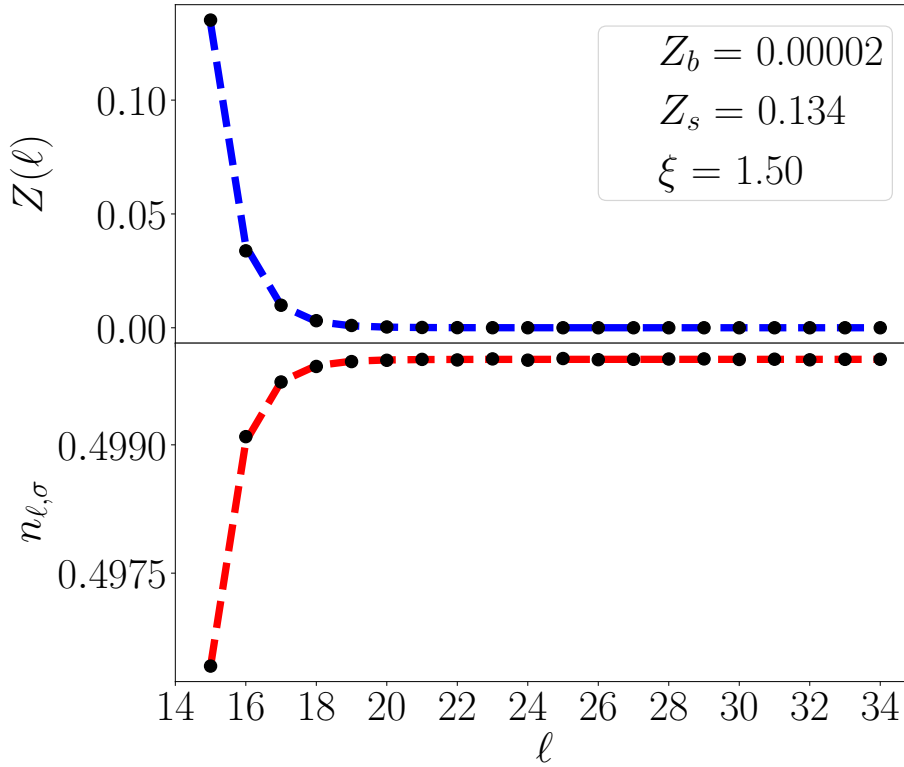


Figure 5: Spatial profile of the quasiparticle residue and electron density per spin across the layers. The last metallic layer is placed at $\ell = 14$. The Hubbard repulsion in the metal layers is $U = 2$ and in the insulating ones $U = 16.828$, and $\delta\mu = -0.9$. The dashed line in the top panel is obtained by the fit. On the contrary, the dashed line in the bottom panel is obtained through (A.6) in Appendix A.2. The legend shows the parameters obtained by the fit, where $Z_s = R_s^2$ and $Z_b = R_b^2$ are the value of the metallicity in the first insulating layer and deep in the bulk.

by simulating a metal-Mott interface away from p-h symmetry. More specifically, we study a system of 100 layers where 15 layers are metallic with $U = 2$, the value that we use here and in the next section. In Fig. 5 we plot the layer-dependent quasiparticle residue and the electron density per spin starting from the last metallic layer and for $\delta\mu = -0.9$, see Eq. (38). Differently from the p-h symmetric case, the proximity effect is shown also in the electron density, which is no longer constrained by p-h symmetry. We fit the layer dependent wavefunction renormalization through the expression:

$$R(\ell) = R_b + (R_s - R_b) e^{(\ell - \ell_*)/\xi}, \quad (47)$$

where ℓ_* is the index of the first insulating layer and ξ the correlation length. From equation (47) we can obtain the quasiparticle residue, which in standard Gutzwiller is just $Z(\ell) = R(\ell)^2$. Instead, the functional form of the density can be deduced, near criticality, by (47) through equation (A.6) in Appendix A.2. For $\delta\mu = -0.9$, the first-order Mott transition occurs at $U_c \approx 16.3$, and ξ diverges as $1/\sqrt{|U - U_c|}$ approaching the transition, a typical mean-field exponent. To further confirm the critical properties of the wetting layer, we rescale both the layer coordinate and $Z(\ell)$ as discussed in [95]. Indeed, all data for different values of U collapse on the same curve, as shown in Fig. 6, supporting the wetting critical behavior, see also Appendix A.2.

3.3 Ghost Gutzwiller results

We can readily extend the results of the previous section to the ghost-GA approximation. In the bulk case and for the single band Hubbard model, it has been shown [9] that already with $N_{aux} = 3$ one can obtain the Hubbard bands and have a quantitative description of the Mott transition in excellent agreement with the DMFT solution.

We find that moving away from p-h symmetry the transition within ghost-GA remains second-order, even upon increasing the number of auxiliary fermions, as discussed in section 3.4. We are therefore back to the surface critical behavior discussed in [95, 97]. We study systems up to 30 layers with $N_{aux} = 3$ and find a clear proximity effect both in the quasiparticle residue and the electron density, as shown in Fig. 7. Besides uncovering, as before, the critical behavior, we can now examine how the presence of the metallic leads affects the quasiparticles in the insulating layers. In Fig. 8, we show the quasiparticle bands along high-symmetry paths of the two-dimensional Brillouin zone, corresponding to the y - z plane, in the case with 10 metallic layers out of 30. We observe the following qualitative structure of the figure: some bands cross zero energy, corresponding to the metallic layers, and the others accumulate to form lower and upper Hubbard bands. In particular, a

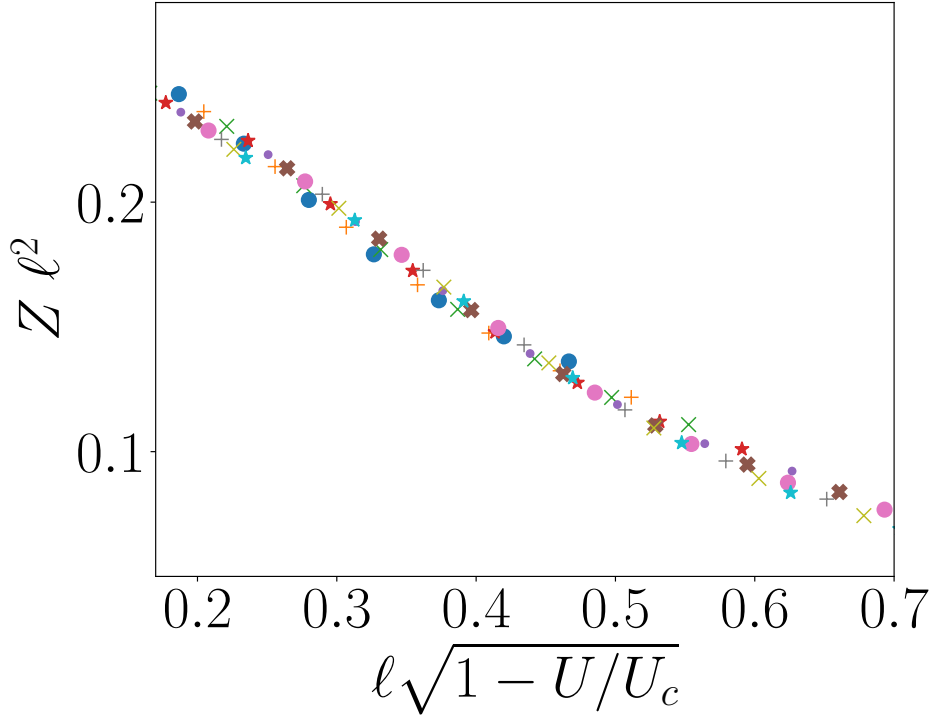


Figure 6: Scaling plot for the quasiparticle residue at $\delta\mu = -0.9$ close to the critical point confirming the mean field exponent $\nu = 1/2$.

feature that we always find is a set of flat bands pinned at zero energy. We shall thoroughly discuss these zero-energy modes in the Sec. 3.4, but we anticipate here that they essentially describe spinons, i.e., gapless spin-1/2 neutral excitations. What is remarkable in Fig. 8 is that the spinon band does not shift rigidly with $\delta\mu$ in Eq. (38), as the Hubbard bands instead do, but remains pinned at zero energy, i.e., the location of the chemical potential.

The spinons thus offer a very simple interpretation of the Kondo proximity effect: at the interface with the metal the spinon reacquires charge and gets promoted into a Kondo resonance narrowly peaked at zero energy. More precisely, the flat band hybridizes with the last metallic layer like in heavy fermion systems, leading to a very narrow band and the opening of small hybridization gaps. To motivate this claim we plot in figure 9 the layer character of the low energy bands of figure 8, showing how the first insulating layer contributes to the dispersive bands. For completeness, in Fig. 10 we plot the layer-resolved spectral function $\mathcal{A}(\omega, \ell) = -\text{Im } G(\omega, \ell) / \pi$ for a slab made of five metallic and five insulating layers that further highlights the layer evolution of the Kondo peak. We have thus shown that the zero-energy quasiparticle excitations inside the paramagnetic Mott insulator,

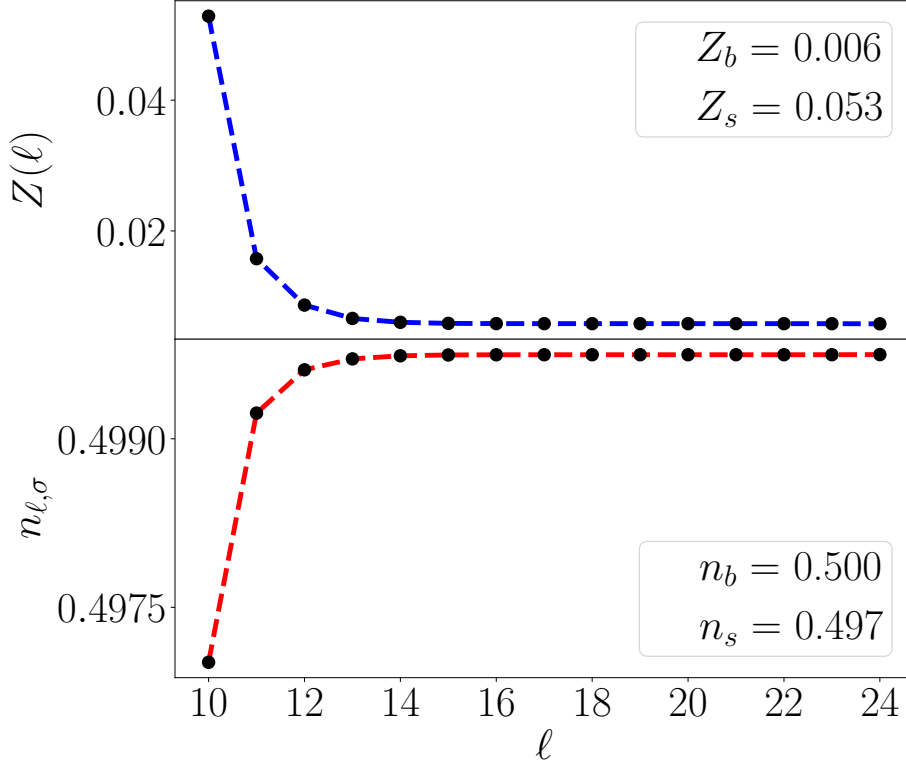


Figure 7: Behaviour of the ghost-GA quasiparticle residue and electron density per spin at $\delta\mu = -0.5$, using $U = 14.385$ in the insulating layers. The last metallic layer is $\ell = 9$. In the legends are reported the quasiparticle residue and the density in the bulk (Z_b, n_b) and in the first insulating layer (Z_s, n_s).

a simple version of a quantum spin liquid, appear at metallic interfaces in the form of a heavy-fermion proximity effect.

A striking experimental counterpart of this doping-independent pinning was recently reported for the paramagnetic Mott insulator Ca_2RuO_4 . Surface doping by alkali-metal adsorption (electron-like) and by C_{60} adsorption (hole-like) both create a coherent in-gap state pinned at the chemical potential, with no gap-crossing jump as the doping polarity is reversed [55, 56], see Fig. 3 (c). While in the experiment the charge is supplied by adatoms rather than by a metal lead, this ambipolar pinning is exactly what is expected if the in-gap state originates from a neutral mode that only borrows charge symmetrically from whatever reservoir it is coupled to, lending qualitative support to our identification of the $\delta\mu$ -independent flat band as the spinon mode. Indeed, it was shown in [56] that the peak positions of the Cs- and C_{60} -dosed cases are quantitatively comparable, suggesting a common origin of the peak that emerges after dopant deposition. Specifically, a coherent quasiparticle forms close to the Fermi level, lying inside the Mott gap in the pristine system and positioned asymmetrically between the two Hubbard bands, just as in

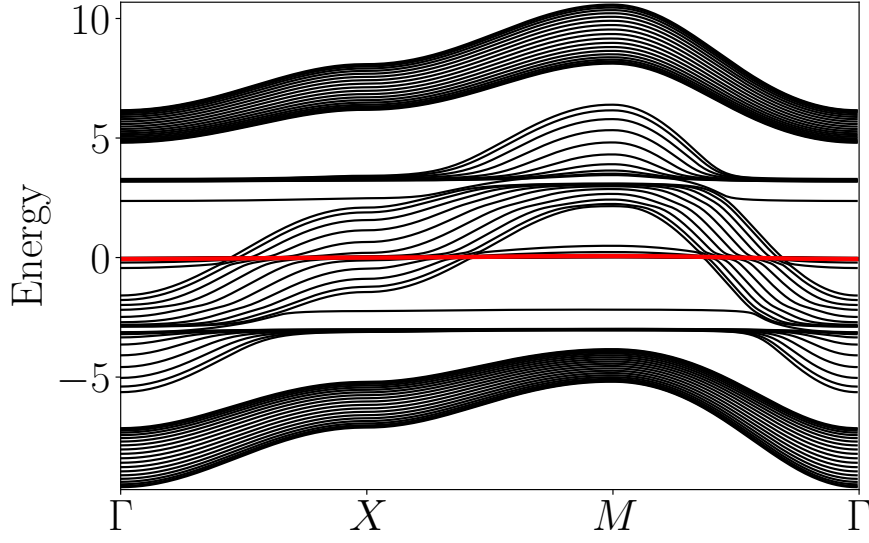


Figure 8: Bands of the quasiparticle Hamiltonian for a slab with 10 metallic layers and 20 Mott insulating ones, at $\delta\mu = -0.5$ and $U = 15$ in the insulating layers.

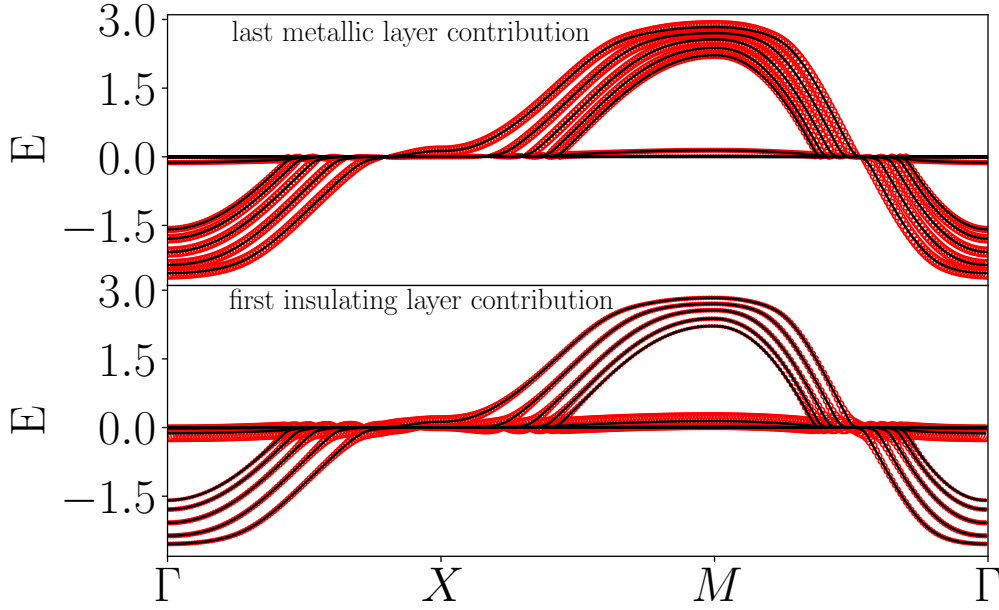


Figure 9: The layer-resolved bands of Fig. 8 at low energy, where the size of the red circles is proportional to the contribution of the corresponding layer. Top panel: contribution of the last metallic layer. Bottom panel: contribution of the first insulating layer. We observe that the flat band of the insulating layer acquires a finite dispersion through the hybridization with the neighboring metallic one.

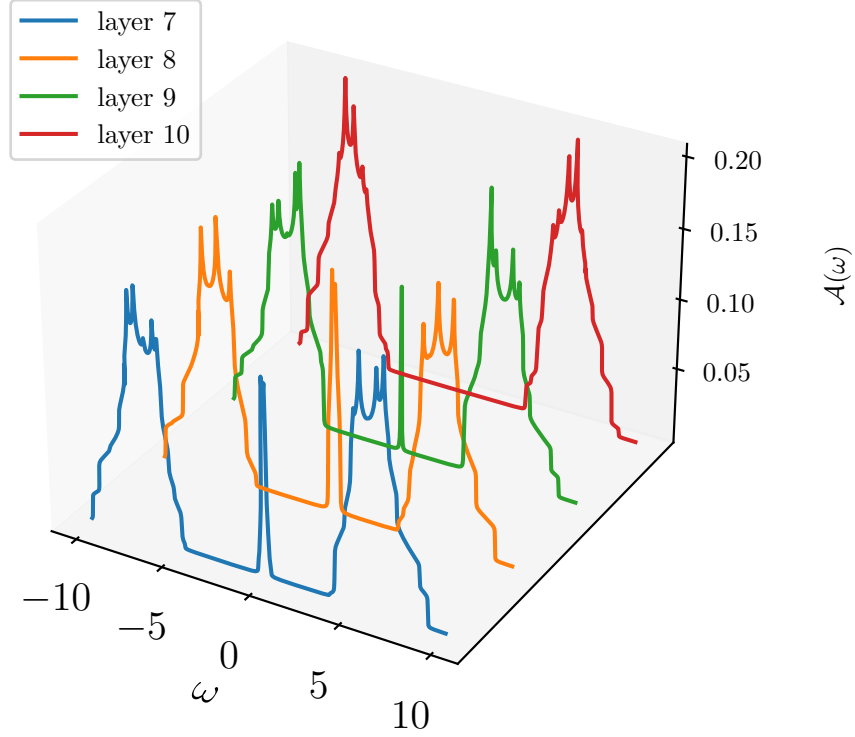


Figure 10: Layer resolved spectral function for $\delta\mu = 0.5$ and $U = 14.316$ showing how the Kondo peak, always centred at zero frequency, disappears moving away from the interface.

our quasiparticle band structure. We believe that the charge-neutral spinon mode gaining charge from the contact with a metallic bath is a natural explanation for this phenomenon.

3.4 Origin of the spinon mode

In this section, we highlight by simple analytical calculations the role played by the zero-energy quasiparticles in the variational optimization, and show that they possess all prerequisites for being legitimately regarded as *spinons*. Consistently with the slab geometry in Fig. 4, we consider a bulk system on a cubic lattice with periodic boundary conditions.

We start by showing that in ghost-GA the Mott transition is second order also away from p-h symmetry, unlike in GA or DMFT. In Fig. 11 we show the evolution of the energy, average density per spin and quasiparticle residue, first upon increasing U from the weakly correlated metal (blue solid lines), and then decreasing it from the insulating side (red dashed lines). We observe a metal-insulator coexistence, but, differently from DMFT away from p-h symmetry, the energy does not show any

discontinuity in the slope as expected at a first order phase transition. Rather, the behavior in Fig. 11 resembles the DMFT one at p-h symmetry [96], where there is metal-insulator coexistence but the metal spinodal point coincides with the value of U at which the two energies cross, hence the accidental second-order transition. We mention that a similar disagreement between ghost-GA and DMFT was observed in [99] studying the Mott transition in the presence of a magnetic field, which is predicted continuous in ghost-GA and discontinuous in DMFT. Another feature of the bulk ghost-GA solution, in common with the previous slab geometry, is that the quasiparticle bands include dispersing and p-h asymmetric lower and upper Hubbard bands, as well as a flat band pinned at zero energy in the Mott phase that reacquires a narrow dispersion in the correlated metal, see Fig. 12.

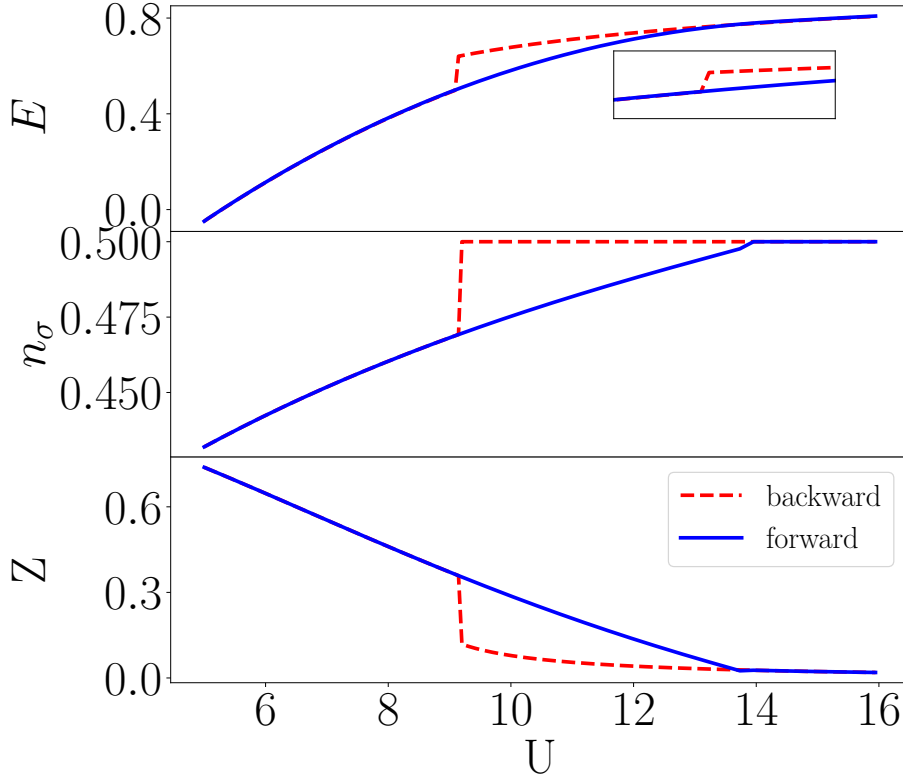


Figure 11: Ground state energy, quasiparticle residue, and density per spin as a function of U in the cubic lattice Hubbard model at $\delta\mu = -1$.

3.4.1 Paramagnetic solution

To enlighten the role of the zero-energy quasiparticles, we here elaborate on the arguments presented in [99], see also [115]. Specifically, we consider the embedded impurity model with $N_{aux} = 3$, sketched in Fig. 13. The impurity level is on the right,

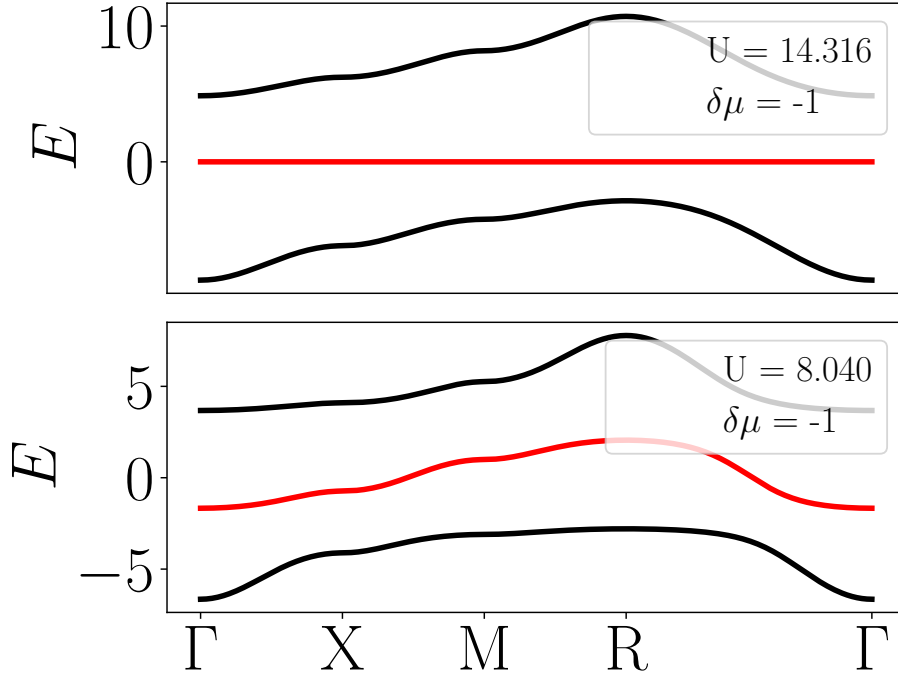


Figure 12: Bands of the quasiparticle Hamiltonian drawn along high-symmetry paths in the Brillouin zone of a cubic lattice for $\delta\mu = -1$. The top panel refers to $U = 14.316$ in the Mott insulating phase, while the bottom panel to $U = 8.040$ in the correlated metal with preformed Hubbard bands.

in blue, shifted up in energy by $-\delta\mu$, with $\delta\mu < 0$ in the figure. In the Mott insulator, U overwhelms by far $\delta\mu$ so that the impurity wants to be half-filled, in the figure with a spin-up electron. The positive-energy and negative-energy bath levels, in red, correspond, respectively, to the lower (LHB) and upper (UHB) Hubbard bands, and are hybridised with the impurity by V_{LHB} and V_{UHB} . The bath level in between, in black, is instead not hybridised with the impurity [9]. At order zero in V_{LHB} and V_{UHB} , the LHB is full and the UHB empty, as in the figure. However, because of the finite hybridisation, the actual ground state of the impurity+LHB+UHB model, in cyan in Fig. 13, includes other configurations, for instance the impurity empty and one electron on the UHB. We remark that, to maximise the energy gain of the hybridisation, it is preferable that the LHB and UHB are symmetrically located with respect to the impurity level, thus both shifted by $-\delta\mu$, as in the figure.

We denote as $|\Psi_\sigma\rangle$ the actual ground state of the impurity+LHB+UHB model, where $\sigma, \uparrow$ in the figure, is the z -component of the total spin, which is $1/2$ in the ground state. One may naïvely argue that the decoupled bath level is fully irrelevant and can be in any configuration, singly occupied, empty or doubly occupied. This is not true however, since Eq. (45) connects the single-particle reduced density matrix of the bath levels with the local single-particle density matrix of the quasiparticles,

which, in turn, affects the expectation value of $\mathcal{H}_*$ in Eq. (40). One can readily convince oneself that the lowest variational energy is obtained with the decoupled bath level singly-occupied and coupled in a spin-singlet configuration with the impurity+LHU+UHB or, in other words, the wavefunction

$$|\phi\rangle = \frac{1}{\sqrt{2}} (|\psi_\uparrow\rangle |\Psi_\downarrow\rangle - |\psi_\downarrow\rangle |\Psi_\uparrow\rangle). \quad (48)$$

Indeed, let us denote the Fock states of a single level as $\gamma = 0$, the empty state,

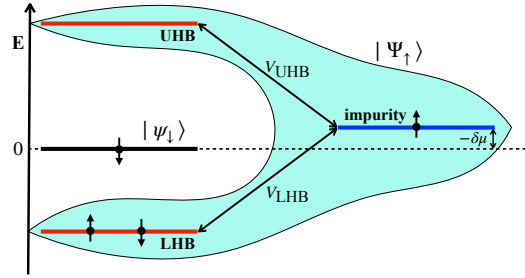


Figure 13: Schematic representation of the effective impurity model in the Mott insulator.

$\gamma = \sigma$, the state with a spin- σ electron, and $\gamma = 2$, the doubly occupied one, and the Fock states of the impurity+LHB+UHB as $|\gamma_{imp}, \gamma_{LHB}, \gamma_{UHB}\rangle$. For large U , we can safely assume the trial wavefunction

$$|\Psi_\sigma\rangle = \cos \theta |\sigma, 2, 0\rangle + \frac{\sin \theta}{\sqrt{2}} (|0, 2, \sigma\rangle + |2, \sigma, 0\rangle), \quad (49)$$

with $\theta \simeq 0$. Using the spin-singlet configuration in Eq. (48), we find that the occupation numbers of LHB and UHB are spin-independent and read

$$n_{LHB\sigma} = 1 - \frac{1}{4} \sin^2 \theta, \quad n_{UHB\sigma} = \frac{1}{4} \sin^2 \theta, \quad (50)$$

while the impurity is half-filled. We note that Eq. (45) entails that the quasiparticle local density matrix is the p-h transform of the impurity bath one, thus that the impurity LHB and UHB transform, respectively, into the quasiparticle UHB and LHB. Since, for $a = \text{LHB, UHB}$,

$$\langle \phi | d_{a\sigma}^\dagger c_\sigma | \phi \rangle = \frac{\sin \theta \cos \theta}{2\sqrt{2}}, \quad (51)$$

and $n_{a\sigma}(1 - n_{a\sigma}) = \sin^2 \theta / 4$ are independent of a , the wavefunction renormalization factors are as well, and read [9]

$$R_{a\sigma} = \frac{\langle \phi | d_{a\sigma}^\dagger c_\sigma | \phi \rangle}{\sqrt{n_{a\sigma}(1 - n_{a\sigma})}} = \frac{2}{\sin \theta} \frac{\sin \theta \cos \theta}{2\sqrt{2}} \simeq \frac{1}{\sqrt{2}}.$$

The quasiparticle Hamiltonian Eq. (43) is therefore

$$\begin{aligned}\mathcal{H}^{qp} &= \frac{1}{2} \sum_{\mathbf{k}\sigma} \sum_{a,b=\text{LHB,HUB}} \epsilon(\mathbf{k}) d_{\mathbf{k}a\sigma}^\dagger d_{\mathbf{k}b\sigma} - \lambda \sum_{\mathbf{k}} (n_{\mathbf{k}\text{LHB}} - n_{\mathbf{k}\text{UHB}}) \\ &= \mathcal{H}_* - \lambda \sum_{\mathbf{k}} (n_{\mathbf{k}\text{LHB}} - n_{\mathbf{k}\text{UHB}}),\end{aligned}\quad (52)$$

plus the flat zero-energy band that, because of Eq. (45) and Eq. (48), is half-filled with equal number of spin up and down quasiparticles. The Hamiltonian in Eq. (52) describes two bands with dispersion

$$\epsilon_{\mp}(\mathbf{k}) = \frac{1}{2} \left(\epsilon(\mathbf{k}) \mp \sqrt{\epsilon(\mathbf{k})^2 + 4\lambda^2} \right),$$

and corresponding eigenoperators

$$\begin{aligned}d_{\mathbf{k}-\sigma} &= \cos \theta_{\mathbf{k}} d_{\mathbf{k}\text{LHB}\sigma} + \sin \theta_{\mathbf{k}} d_{\mathbf{k}\text{UHB}\sigma}, \\ d_{\mathbf{k}+\sigma} &= -\sin \theta_{\mathbf{k}} d_{\mathbf{k}\text{LHB}\sigma} + \cos \theta_{\mathbf{k}} d_{\mathbf{k}\text{UHB}\sigma},\end{aligned}\quad (53)$$

with $\tan 2\theta_{\mathbf{k}} = \epsilon(\mathbf{k})/2\lambda$. The parameter λ in Eq. (52) is a Lagrange multiplier that enforces the self-consistency condition in Eq. (45), namely, that the LHB is almost full and the HUB almost empty. This requires $\lambda \gg t$, thus $\epsilon_{-}(\mathbf{k}) < 0$ and $\epsilon_{+}(\mathbf{k}) > 0$ separated by a gap 2λ , and the ground state $|\Psi_*\rangle$ obtained by filling the lowest-energy band. Specifically, the self-consistency Eq. (45) together with Eq. (50) imply, through Eq. (53), that

$$\begin{aligned}\frac{1}{V} \sum_{\mathbf{k}} \langle \Psi_* | n_{\mathbf{k}\text{LHB}} | \Psi_* \rangle &\simeq 2 - \frac{3t^2}{4\lambda^2} = 2 - \frac{\sin^2 \theta}{2}, \\ \frac{1}{V} \sum_{\mathbf{k}} \langle \Psi_* | n_{\mathbf{k}\text{UHB}} | \Psi_* \rangle &\simeq \frac{3t^2}{4\lambda^2} = \frac{\sin^2 \theta}{2}.\end{aligned}$$

It follows that $3t^2/2\lambda^2 = \sin^2 \theta$ and that the variational energy per site is

$$\begin{aligned}E &= \frac{1}{V} \langle \Psi_* | \mathcal{H}_* | \Psi_* \rangle + \frac{U}{2} \langle \phi | (n-1)^2 | \phi \rangle \\ &\simeq -\frac{3t^2}{\lambda} + \frac{U}{2} \sin^2 \theta = -\frac{3t^2}{\lambda} + \frac{U}{2} \frac{3t^2}{2\lambda^2},\end{aligned}$$

with minimum at $\lambda = U/2$ and value $E = -3t^2/U$. We recall that the half-filled Hubbard model at very large U maps onto a spin-1/2 Heisenberg model

$$H_{\text{Heis}} = J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right), \quad (54)$$

where $J = 4t^2/U$. We realize that on a cubic lattice the large- U ghost-GA variational energy per site, $E = -3t^2/U$, actually $E = -zt^2/2U$ for generic lattices with

coordination number z , reproduces the second term in parenthesis. This represents a big achievement with respect to the standard GA, which yields a vanishing variational energy [60], and is consistent with the fact that ghost-GA is strictly variational for lattices with infinite coordination, where the term $S_i \cdot S_j$ does not contribute unless breaking the spin $SU(2)$.

In other words, the self-consistency condition Eq. (45) effectively provides a strong spin entanglement [99] between the impurity+LHU+UHB and the decoupled bath level, which is forced to lie at zero energy, thus yielding the zero-energy quasiparticle flat-band that, we argue, hosts the spinons. In the next Chapter, we will show how to systematically improve this result valid at strong coupling to obtain an impurity wavefunction that provides a description of the system valid in the whole range of parameter U for which we have a Mott insulator.

3.4.2 Ferromagnetic solution

To support the conjecture of strong spin entanglement between the impurity+LHU+UHB and the decoupled bath level, let us study a ghost-GA variational wavefunction with finite magnetisation m per site. Instead of Eq. (48), see Eq. (49), we use as trial wavefunction for the impurity state

$$|\phi\rangle = \cos\theta \cos\phi |\psi_\downarrow\rangle |\uparrow, 2, 0\rangle - \cos\theta \sin\phi |\psi_\uparrow\rangle |\downarrow, 2, 0\rangle + \frac{\sin\theta}{2} |\psi_\downarrow\rangle (|0, 2 \uparrow\rangle + |2, \uparrow, 0\rangle) - \frac{\sin\theta}{2} |\psi_\uparrow\rangle (|0, 2 \downarrow\rangle + |2, \downarrow, 0\rangle), \quad (55)$$

which allows for a finite impurity magnetisation that corresponds to the physical one m , thus $n_\uparrow - n_\downarrow = \cos 2\phi \cos^2 \theta = m$. We note that the magnetisation of the decoupled bath level coincides with $-m$, which shows that the physical spin is entirely carried by the zero-energy states in the quasiparticle Hamiltonian, whose magnetisation is the p-h transform of the decoupled bath level, thus precisely m . Indeed, the choice in Eq. (55) is intentionally made with that purpose. We have confirmed that it reproduces the numerically optimized solution. Correspondingly, the occupation numbers of the LHB and UHB are the same as in Eq. (50), i.e., spin independent. What changes are the expectation values in Eq. (51), which now read

$$\begin{aligned} \langle\phi| d_{\text{UHB}\uparrow}^\dagger c_\uparrow |\phi\rangle &= \langle\phi| d_{\text{LHB}\downarrow}^\dagger c_\downarrow |\phi\rangle = \cos\phi \frac{\sin\theta \cos\theta}{2}, \\ \langle\phi| d_{\text{LHB}\uparrow}^\dagger c_\uparrow |\phi\rangle &= \langle\phi| d_{\text{UHB}\downarrow}^\dagger c_\downarrow |\phi\rangle = \sin\phi \frac{\sin\theta \cos\theta}{2}, \end{aligned} \quad (56)$$

resulting in the following wavefunction renormalization factors

$$R_{\text{UHB}\uparrow} = R_{\text{LHB}\downarrow} \simeq \cos\phi, \quad R_{\text{LHB}\uparrow} = R_{\text{UHB}\downarrow} \simeq \sin\phi. \quad (57)$$

The consequence, as one can readily derive following the former calculations at $m = 0$, is a reduction of

$$\langle \Psi_* | \mathcal{H}_* | \Psi_* \rangle \simeq -\frac{3t^2}{\lambda} \sin^2 2\phi,$$

and a modified self-consistency condition

$$\frac{3t^2}{2\lambda^2} = \frac{\sin^2 \theta}{\sin^2 2\phi},$$

both of which reduce to the previous ones when $\phi = \pi/4$. The variational energy per site is therefore

$$E = -\frac{3t^2}{\lambda} \sin^2 2\phi + \frac{U}{2} \sin^2 \theta = -3t^2 \sin^2 2\phi \left(\frac{1}{\lambda} - \frac{U}{4\lambda^2} \right),$$

with the constraint

$$m = \cos 2\phi \cos^2 \theta = \cos 2\phi \left(1 - \frac{3t^2}{2\lambda^2} \sin^2 2\phi \right) \xrightarrow{\lambda \gg t} \cos 2\phi,$$

from which we find that the optimal $\lambda = U/2$, as before, and

$$E(m) = -\frac{3t^2}{U} (1 - m^2). \quad (58)$$

We note that Eq. (58) corresponds precisely to the expectation value per site of the Heisenberg Hamiltonian in Eq. (54) over a state with average spin polarization $\langle S_i^z \rangle = m/2$ in the limit of infinite coordination-number. In other words, in this limit the variational ghost-GA wavefunction reproduces the exact ground state energy and it does so in a very physical way: the spin polarization is carried just by the quasiparticles of the flat band, justifying our interpretation of them as *spinons*, whereas the dispersive Hubbard bands remain unpolarized.

We further observe that, even though the spinon band is flat in the quasiparticle Hamiltonian, the variational energy in Eq. (58) is instead compatible with a non-zero dispersion and a finite spinon density-of-states at zero energy. The reason lies in the fact that the spinon and Hubbard bands are not truly independent of each other. Indeed, the spinon polarization does affect the Hubbard bands through (57), and, in turn, the expectation value $\langle \Psi_* | \mathcal{H}_* | \Psi_* \rangle$. This behavior is similar to the outcome of conventional Hartree-Fock plus random-phase approximation, and suggests that the inclusion of quantum fluctuations, as done for the GA using the time-dependent variational principle [61], may explicitly unveil the coupling between the Hubbard bands and the spinon one. In that case, a finite spinon dispersion should appear upon integrating out the high-energy Hubbard bands. Moreover, the finite spinon density-of-states consistent with Eq. (58) suggests that the spinons do have a well-defined Fermi-surface.

3.4.3 Antiferromagnetic solution

To conclude this section and provide further evidence of the quality of the variational ghost-GA wavefunction, let us briefly discuss the solution when we allow for antiferromagnetism. On a bipartite lattice with hopping just between the two sublattices, we expect the ground state to describe an antiferromagnetic insulator for any $U > 0$, as mentioned in the Introduction. Let us therefore extend the previous analysis to an antiferromagnet at fixed staggered magnetisation m . We assume that both sublattices, which we denote as A and B, are described by the auxiliary impurity wavefunction (55) with sublattice dependent ϕ , specifically, $\phi_A = \phi$ and $\phi_B = \pi/2 - \phi$, thus opposite sublattice magnetisations

$$m_A = \cos 2\phi \cos^2 \theta \equiv m, \quad m_B = -m. \quad (59)$$

The occupation numbers per spin are still those in (50). The wavefunction renormalizations are the same as in (57) for sublattice A, while $\cos \phi \leftrightarrow \sin \phi$ for sublattice B. It follows that the quasiparticle Hamiltonian (43) in the LHB-UHB orbital space is characterized by uniform diagonal and off-diagonal hopping amplitudes $-t \sin 2\phi/2$ and $-t/2$, respectively, as well as by a staggered off-diagonal hopping $-t \cos 2\phi/2$ due to antiferromagnetism, more details on the quasiparticle Hamiltonian can be found in Appendix D. In addition, the Hamiltonian includes a Lagrange multiplier λ that enforces the self-consistency condition $n_{\text{LHB}} - n_{\text{UHB}} = 2 - \sin^2 \theta$, and one that fixes the local density, $n_{\text{LHB}} + n_{\text{UHB}} = 2$. For $U \gg t$, λ is also large and the quasiparticle Hamiltonian $\mathcal{H}^{qp}$ in the halved, magnetic Brillouin zone (MBZ) describes an insulator with occupied valence bands

$$\begin{aligned} \epsilon_1(\mathbf{k}) &= -\frac{1}{2} \sqrt{2\epsilon(\mathbf{k})^2 + 4\lambda^2 - 2\epsilon(\mathbf{k}) E(\mathbf{k})}, \\ \epsilon_2(\mathbf{k}) &= -\frac{1}{2} \sqrt{2\epsilon(\mathbf{k})^2 + 4\lambda^2 + 2\epsilon(\mathbf{k}) E(\mathbf{k})}, \end{aligned}$$

and empty conduction ones, $\epsilon_3(\mathbf{k}) = -\epsilon_2(\mathbf{k})$ and $\epsilon_4(\mathbf{k}) = -\epsilon_1(\mathbf{k})$, where $E(\mathbf{k}) = \sqrt{\epsilon(\mathbf{k})^2 + 4\lambda^2 \sin^2 2\phi}$. The constraint $n_{\text{LHB}} + n_{\text{UHB}} = 2$ is therefore automatically satisfied. Concerning the other constraint, if

$$E^{qp}(\lambda) = \frac{2}{V} \sum_{\mathbf{k} \in \text{MBZ}} (\epsilon_1(\mathbf{k}) + \epsilon_2(\mathbf{k})) \simeq -2\lambda - (1 + \cos^2 2\phi) \frac{3t^2}{2\lambda},$$

is the ground state energy per site of $\mathcal{H}^{qp}$, the last equation being valid for $\lambda \gg t$ on a cubic lattice, we have to impose that

$$n_{\text{LHB}} - n_{\text{UHB}} = 2 - \sin^2 \theta = -\frac{\partial E^{qp}(\lambda)}{\partial \lambda} \simeq 2 - (1 + \cos^2 2\phi) \frac{3t^2}{2\lambda^2},$$

thus

$$\sin^2 \theta = (1 + \cos^2 2\phi) \frac{3t^2}{2\lambda^2},$$

and

$$\frac{1}{V} \langle \Psi_* | \mathcal{H}_* | \Psi_* \rangle = E^{qp}(\lambda) + \lambda (n_{\text{LHB}} - n_{\text{UHB}}) \simeq -\frac{3t^2}{\lambda} (1 + \cos^2 2\phi).$$

Performing the same steps as in the ferromagnetic case, we finally get a variational energy per site that reads, in the general case of a d -dimensional hypercubic lattice,

$$E_{\text{AF}}(m) = -\frac{dt^2}{U} (1 + m^2), \quad (60)$$

which decreases with $|m|$, showing that the paramagnetic solution at $m = 0$ is unstable towards developing an antiferromagnetic order parameter. Moreover, (60) coincides with the ground state energy of (54) at fixed staggered magnetisation m for large d , i.e., when quantum fluctuations can be ignored. As before, the staggered magnetisation is carried solely by the spinons, the flat-band quasiparticles, while the Hubbard bands are spin unpolarised. This is in sharp contrast with the Hartree-Fock approximation, where the staggered magnetisation is due to the valence and conduction bands that mimic, within Hartree-Fock approximation, the Hubbard bands, and are separated from each other by a gap $\sim 2Um$ instead of the expected U , the actual cost of a charge excitation.

Whether this provides a much better description of the large U antiferromagnetic insulator than, e.g., the Hartree-Fock approximation, is a question that we will answer in the next Chapter.

3.5 Conclusions

We have shown that the ghost Gutzwiller approximation is able to describe a genuine paramagnetic Mott insulator that hosts neutral spin-1/2 quasiparticles, possibly with their own Fermi surface, the sought-after Anderson's spinons. Specifically, the spin-singlet wavefunction of the auxiliary impurity model implies that the linear operator $\mathcal{P}_G$ in (39) is spin $SU(2)$ invariant. The spin state of the full ghost Gutzwiller wave function thus depends on the spin state of the Slater determinant in Eq. (39), which our results suggest to be a singlet. Indeed, the contribution of the Hubbard bands to the Slater determinant is trivially a spin-singlet state, since they are either completely full or empty. While the energy optimization does not completely determine the spinon contribution to the Slater determinant, as it appears with its corresponding R equal to zero, we know that this term is characterized by an $SU(2)$ -invariant local density matrix, fixed by the ghost Gutzwiller self-consistency. We believe that these observations, together with the finite paramagnetic susceptibility entailed by (58), collectively provide evidence that the optimal ghost-Gutzwiller wavefunction in the Mott phase is indeed a global spin singlet with gapless spinons.

Furthermore, we have demonstrated that these spinons can be revealed by a proximity effect at the interface between the paramagnetic Mott insulator and a metal. Indeed, the spinons near the interface regain the electron charge and get promoted into bona fide quasiparticles with a narrow dispersion in the directions parallel to the interface that decreases exponentially moving inside the bulk of the Mott insulator. This behavior is more akin to a heavy-fermion proximity effect than to the Kondo-like one that was advocated to interpret the DMFT results [95].

Lastly, we have shown that when the system is allowed to have a finite magnetization m , the quadratic rise of the energy with m is compatible with the spinons having a finite density of states, hence a finite dispersion in the Brillouin zone, not accessible at $m = 0$.

To unveil the precise form of the spinon dispersion one needs to include quantum fluctuations on top of the variational solution. The inclusion of quantum fluctuations in the ghost Gutzwiller approximation can be done through the time-dependent variational principle as this would give access to correlation functions by expanding the action to second order in the fluctuations around the saddle point, similarly to what has been done for the standard Gutzwiller approximation [61]. Recently, the time-dependent variational principle has been applied to the ghost Gutzwiller approximation in the context of the Mott transition [107], showing results in excellent agreement with exact DMFT calculations using real-time diagrammatic Monte Carlo as an impurity solver. These results are promising and suggest that the time-dependent variational principle can be used to unveil the spinon dispersion in the Mott insulator.

4

DIRECT MINIMIZATION VERSUS ITERATIVE EMBEDDING IN THE GHOST-GUTZWILLER METHOD: A COMPARATIVE STUDY OF MAGNETISM IN MOTT INSULATORS

As mentioned in Chapter 2, the ghost-Gutzwiller method can be solved either through an iterative embedding scheme, similar to dynamical mean-field theory, or by directly minimizing the energy functional by optimizing the impurity wavefunction.

This flexibility presents an opportunity to address a longstanding challenge in iterative quantum embedding methods: accurately describing a hypothetical symmetry-invariant Mott insulator.

We demonstrate that, across the Mott transition of the single-band Hubbard model, these two formally equivalent approaches exhibit distinct behaviors. The iterative scheme is computationally efficient but prone to fragility, requiring ad-hoc recipes that may fail in specific situations, such as the presence of a Zeeman field. In contrast, direct minimization avoids these artifacts, stabilizing a Mott insulator with a genuine paramagnetic response to the Zeeman field.

When symmetry breaking is permitted, as in an antiferromagnetic phase, the iterative scheme yields the correct solution, closely aligning with dynamical mean-field theory.

Our findings provide insights into the conditions under which the iterative embedding method can be trusted and when direct minimization is instead necessary.

The current theoretical understanding of correlated phenomena in condensed matter physics is grounded in self-consistent methods where, typically, the many-body problem is approximated by a simpler, non-linear model that is often solved iteratively, such as the Hartree-Fock approximation. A broad class of self-consistent methods known as quantum embedding theories (QE) [64] partition the original complex problem into a fragment, referred to as the *impurity*, and its environment that are treated at different levels of accuracy, with the impurity being analyzed with greater precision. The coupling between environment and impurity is enforced by particular self-consistency conditions that distinguish the various embedding theories.

A paradigmatic quantum embedding method is DMFT [4]. As mentioned in the previous Chapters, DMFT is exact in lattices with infinite coordination number and with local interactions, but it serves as a sensible approximation in realistic lattices, providing insightful results about correlated phenomena, particularly the Mott

transition. Although DMFT can be formulated through an appropriate functional whose saddle point yields the single-particle Green's function [13, 116], in practice, the self-consistency equation is commonly solved iteratively. The iteration scheme is computationally very convenient, but hinders the enforcement of symmetries that are spontaneously broken in the actual low-temperature state. A prominent example is the paramagnetic Mott insulating state of the half-filled Hubbard model, which stands as one of the key achievements of DMFT. Indeed, to prevent antiferromagnetism, which is known to occur at low temperatures, one must force the convergence of the iterative method through ad hoc recipes of spin symmetrization, as explained in the previous Chapter. This is equivalent to employing a mixed state instead of a pure one, and may be responsible for the residual $\ln 2$ entropy per site of the $T = 0$ Mott insulator found in DMFT. Conversely, one might anticipate that the entropy of the free local moments could be quenched at zero temperature, even in the absence of symmetry breaking, due to the formation of a hypothetical spin-liquid state.

Conventionally, spin liquids are described using Heisenberg-type Hamiltonians, where the charge is frozen right from the outset. However, the substantial number of candidate spin-liquid materials [117–119] makes it worthwhile to explore the interplay between charge and spin dynamics, as it might be relevant to the description of interesting phenomena, such as the one discussed in Chapter 3. Quantum embedding theories, such as DMFT, hold genuine potential to address this issue. Nevertheless, these methods currently struggle to account for the strong frustration and massive spin entanglement [7] that characterize spin-liquids, which can only be described by artificially forcing $SU(2)$ symmetry. As mentioned earlier, this enforcement is challenging in iterative schemes. Here, we show how this problem can be circumvented using ghost-GA.

4.1 Remarks on the difference between the two optimization schemes

The two distinct methods to optimize the ghost-Gutzwiller wavefunction (1), the direct minimization approach and the iterative embedding scheme, have been previously introduced in Sections 2.3 and 2.3.1.

In both approaches, the saddle-point equation for $|\psi_*\rangle$ is just the ground-state problem of a non-interacting Hamiltonian. However, the impurity wavefunction $|\phi\rangle$ in the direct minimization method is obtained by solving a non-linear Schrödinger equation because the functional derivative of $\hat{R}(\phi)$ in (25) is not linear in $|\phi\rangle$. Since this non-linear Schrödinger equation still contains an interaction term acting on the

impurity, its solution is highly complex. To address this, it is often simpler to adopt a suitable parametrization of $|\phi\rangle$ and directly optimize its coefficients. It is possible that the resulting $|\phi\rangle$ does not correspond to any ground state of a conventional Anderson impurity model, where the impurity is interacting but the baths are not, and they are only coupled to the impurity through hybridization. This situation would indicate a clear failure of the embedding scheme, where, by construction, $|\phi\rangle$ is the ground state of an Anderson impurity model. In what follows, we investigate this issue in the simple half-filled Hubbard model.

4.2 The paramagnetic Mott transition within ghost-Gutzwiller revisited

In this section, we revisit the paramagnetic Mott transition within the ghost-Gutzwiller approximation, which was also presented in Section 3.4. We specifically focus on the crucial algorithmic steps required to stabilize the solution in the iterative embedding scheme and compare it with the solution obtained through direct minimization.

We begin by analyzing the non-symmetry-breaking solution of the single-band Hubbard model at half-filling and on a bipartite lattice. Although the actual ground state in this case is an antiferromagnetic insulator, it is still intriguing to explore the possibility of describing a hypothetical metastable symmetry-invariant insulator, free from the complexities introduced by the frustration necessary to stabilize a genuine spin liquid.

The model Hamiltonian reads

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) + \frac{U}{2} \sum_i (n_i - 1)^2, \quad (61)$$

where $t = 1$, our unit of energy, is the nearest-neighbor hopping and U the on-site Coulomb repulsion. We consider a Bethe lattice with infinite coordination number, where the GA becomes exact. The non-interacting density of states is semicircular,

$$\mathcal{D}(\epsilon) = \frac{2}{\pi D} \sqrt{1 - \left(\frac{\epsilon}{D} \right)^2}, \quad (62)$$

with $D = 2$ in our units. Hereafter, we fix $N_{\text{aux}} = 3$, so that the impurity model describes an impurity coupled to three bath sites.

We first consider the weakly correlated regime, $U < U_c$, where the system is a renormalized Fermi liquid. Restricting ourselves to the translationally invariant solution, the embedding scheme converges smoothly to a spin-unpolarized state, and the paramagnetic metal is a local minimum of the ghost-GA functional. Within

this regime the impurity wavefunction is a non-degenerate singlet. This is the situation in which the embedding formulation works at its best, and replacing the explicit minimization of the functional by a self-consistent loop is both safe and computationally advantageous.

Upon increasing U , the system undergoes a Mott transition at a critical U_c where the quasiparticle residue,

$$Z = \left(1 - \partial_{\omega} \text{Re}\Sigma(\omega)|_{\omega=0}\right)^{-1}, \quad (63)$$

where $\Sigma(\omega)$ is the self-energy (37) on the real frequency axis, vanishes and the quasiparticle peaked at the chemical potential disappears in the spectral function. Correspondingly, in the impurity model the bath site sitting at the Fermi level, which for $U < U_c$ hybridizes with the impurity site, progressively decouples as $U \rightarrow U_c^-$ and is completely severed from the impurity for $U > U_c$. The impurity is then left coupled only to the two bath sites describing the lower and upper Hubbard bands, LHB and UHB, respectively. Technically, this decoupling shows up in the natural basis as the vanishing of one entry of the renormalization matrix $\hat{R}$; this feature is a hallmark of the Mott phase.

Once the bath at the Fermi level decouples, the impurity ground state becomes degenerate. This same degeneracy extends to the entire spectrum. Its origin lies in the gauge symmetry of the wavefunction (1): completely broken in the metal, it is restored in the Mott phase for the auxiliary fermion corresponding to the zero-energy decoupled bath. Specifically, if $|\phi_{\sigma}\rangle$, $\sigma = \uparrow, \downarrow$, is the spin-1/2 ground-state wavefunction of the impurity plus the two coupled baths, while $|\gamma_1\rangle$ and $|\gamma_2\rangle$ any two orthogonal states of the decoupled bath, then

$$|\phi\rangle = |\phi_{\uparrow}\rangle |\gamma_1\rangle + |\phi_{\downarrow}\rangle |\gamma_2\rangle,$$

yields the same variational energy for any choice of $|\gamma_1\rangle$ and $|\gamma_2\rangle$. Even if we partially fix the gauge by employing physical symmetries, such as imposing that $|\phi\rangle$ is eigenstate of the number of particles with eigenvalue corresponding to half-filling [120], and of S_z with eigenvalue $S_z = 0$, thereby restricting the available states of the decoupled bath to $|\gamma\rangle = |\uparrow\rangle, |\downarrow\rangle$, we are still left with a double degenerate impurity wavefunction

$$|\phi_{\pm}\rangle = |\phi_{\uparrow}\rangle |\downarrow\rangle \mp |\phi_{\downarrow}\rangle |\uparrow\rangle, \quad (64)$$

where $|\phi_{+}\rangle$ is a spin singlet and $|\phi_{-}\rangle$ the $S_z = 0$ component of the spin-triplet. The residual double degeneracy, which corresponds to the Z_2 gauge transformation $|\uparrow\rangle \rightarrow -|\uparrow\rangle$, which is recovered in the Mott phase and is reminiscent of what was discussed in [121], is not removable and is the root cause of a well-known difficulty encountered in the iterative embedding scheme within the Mott phase. This difficulty arises because the impurity ground state selected at each iteration is an uncontrolled linear combination of the two states in (64), thereby hindering the convergence of the scheme, with the impurity magnetization flipping up and down

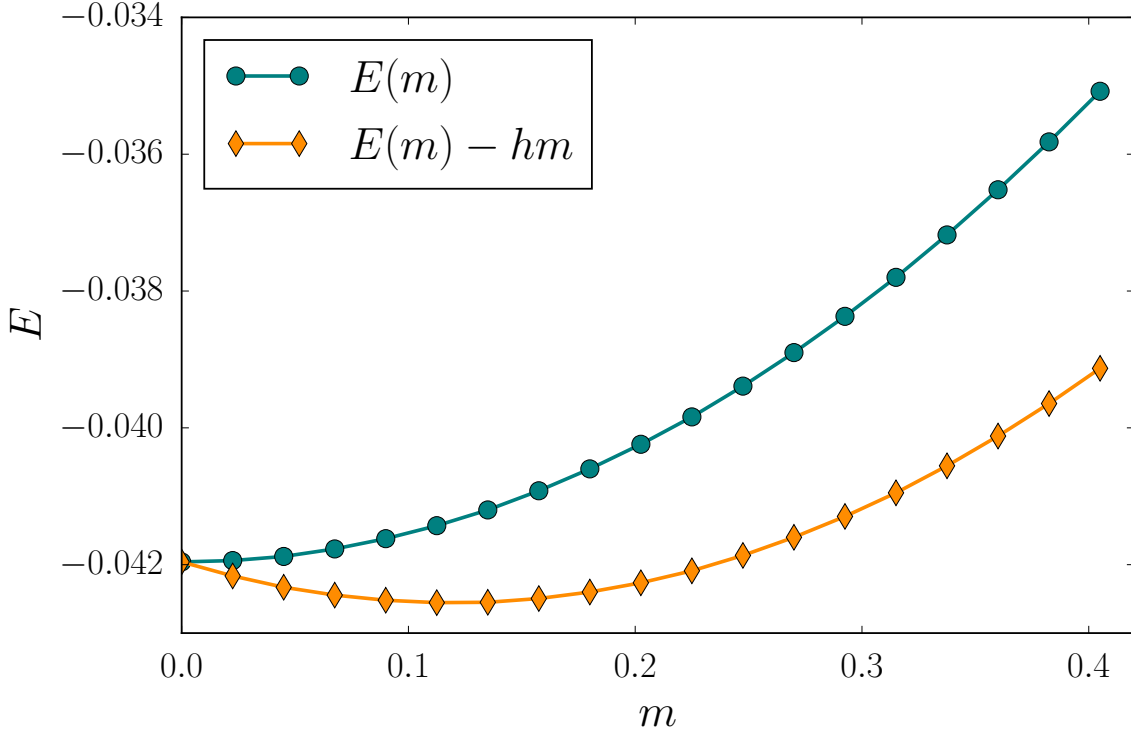


Figure 14: Ghost-GA energy $E(m)$ as a function of the fixed impurity magnetization m , for $U = 12$ in the Mott phase, together with its Legendre transform $E(m) - hm$ in the presence of a magnetic field $h = 0.01$. $E(m)$ is minimum at $m = 0$, confirming that the paramagnetic solution is a local minimum; switching on h shifts the minimum to a finite m .

from one iteration to the next.

A solution to this problem lies in explicitly resolving the degeneracy. Within the twofold degenerate manifold, any state of definite impurity magnetization m can be constructed as a unique linear combination of the two states in (64) [18]. As m approaches zero, the embedding loop converges smoothly to a spin-unpolarized solution. To verify that this is the physically correct choice, we show the ghost-GA energy $E(m)$ as a function of m in Fig. 14 for $U = 12$ in the Mott phase. The energy is minimum at $m = 0$, and it increases monotonically with m .

One might conclude that the Mott phase ambiguity is then solved. The prescription depicted above, however, works only because the two states are exactly degenerate: any perturbation that lifts the degeneracy spoils this construction and results in a completely polarized impurity ground state, at least within the embedding scheme we here consider. This is precisely what happens in a magnetic field, which we discuss in the next Section, and it is expected to occur more generally whenever a perturbation splits the degenerate manifold, as for the crystal-field splitting or the Hund's coupling in multiband models. This motivated us to look for a more robust description of the Mott insulating phase within ghost-GA, i.e., directly minimizing the ghost-GA functional through a suitable parametrization of the

impurity wavefunction $|\phi\rangle$ that encodes the projector $\mathcal{P}_i$.

To this end, we construct the generic impurity wavefunction with a singly-occupied decoupled bath, in the half-filled sector with $S_z = 0$, and with the additional constraints of the coupled baths forming a natural basis, i.e., with a diagonal reduced density matrix, and spin unpolarized. Hence, we generalize the impurity state used at strong coupling in Paragraph 3.4.1. This implies that only the impurity and the decoupled bath may carry magnetic moments, actually opposite to each other because of $S_z = 0$. Practically, we start from the wavefunction

$$|\phi_0\rangle = \cos \varphi |\uparrow, 2, 0\rangle |\downarrow\rangle - \sin \varphi |\downarrow, 2, 0\rangle |\uparrow\rangle, \quad (65)$$

where $|\gamma_{\text{imp}}, \gamma_{\text{LHB}}, \gamma_{\text{UHB}}\rangle |\gamma_{\text{dec}}\rangle$, $\gamma = 0, \uparrow, \downarrow, 2$, are basis states, with $|\gamma_{\text{dec}}\rangle = |\uparrow\rangle, |\downarrow\rangle$ describing the decoupled bath. The angle $\varphi \in [0, \pi/2]$ parametrizes the impurity magnetization, which vanishes at $\varphi = \pi/4$. Next, we generate from (65) a Lanczos chain of states by applying successively the hybridization between the impurity and the high-energy baths, LHB and UHB, forcing the above constraints. At the end, we obtain the impurity wavefunction

$$|\phi\rangle = \sum_{n=0}^4 \alpha_n |\phi_n\rangle, \quad (66)$$

with real α_n satisfying $\sum_n \alpha_n^2 = 1$, where

$$\begin{aligned} |\phi_1\rangle &= \frac{1}{2} \left(|2, \downarrow, 0\rangle |\uparrow\rangle - |2, \uparrow, 0\rangle |\downarrow\rangle - |2, 2, \downarrow\rangle |\uparrow\rangle + |2, 2, \uparrow\rangle |\downarrow\rangle \right), \\ |\phi_2\rangle &= \frac{\sin \varphi}{\sqrt{6}} \left(|\uparrow, \downarrow, \uparrow\rangle |\downarrow\rangle + |\uparrow, \uparrow, \downarrow\rangle |\downarrow\rangle \right) + \frac{\cos \varphi}{\sqrt{6}} \left(|\downarrow, \downarrow, \uparrow\rangle |\uparrow\rangle + |\downarrow, \uparrow, \downarrow\rangle |\uparrow\rangle \right) \\ &\quad - \frac{1}{\sqrt{3}} \left(|\uparrow, \downarrow, \downarrow\rangle |\uparrow\rangle + |\downarrow, \uparrow, \uparrow\rangle |\downarrow\rangle \right), \\ |\phi_3\rangle &= \frac{1}{2} \left(|2, 0, \uparrow\rangle |\downarrow\rangle - |2, 0, \downarrow\rangle |\uparrow\rangle - |0, \uparrow, 2\rangle |\downarrow\rangle + |0, \downarrow, 2\rangle |\uparrow\rangle \right) \\ |\phi_4\rangle &= -\cos \varphi |\uparrow, 0, 2\rangle |\downarrow\rangle + \sin \varphi |\downarrow, 0, 2\rangle |\uparrow\rangle. \end{aligned} \quad (67)$$

Considering the normalization, the wavefunction (66) comprises five free parameters that are optimized by locating the saddle point of (28). More details on the analytical expressions obtained for the ghost-GA functional in the Mott phase are reported in Appendix C. Since (66) incorporates a decoupled bath, it is exclusively suitable for describing the Mott phase and not the correlated metal below U_c .

In Fig. 15 we compare the energies of the embedding scheme obtained through the limit $m \rightarrow 0$, see the above discussion, and the minimization of (66) directly at $m = 0$, i.e., at $\varphi = \pi/4$. As anticipated, the energies deviate below U_c , where (66) is not accurate, but coincide in the Mott regime, $U > U_c$. This both validates our compact ansatz (66) and confirms that the embedding solution, once the degeneracy is correctly resolved, captures the same physics. This agreement holds only in the unperturbed paramagnet; in the next Section, we show that a magnetic field, by lifting the degeneracy, drives the two schemes apart.

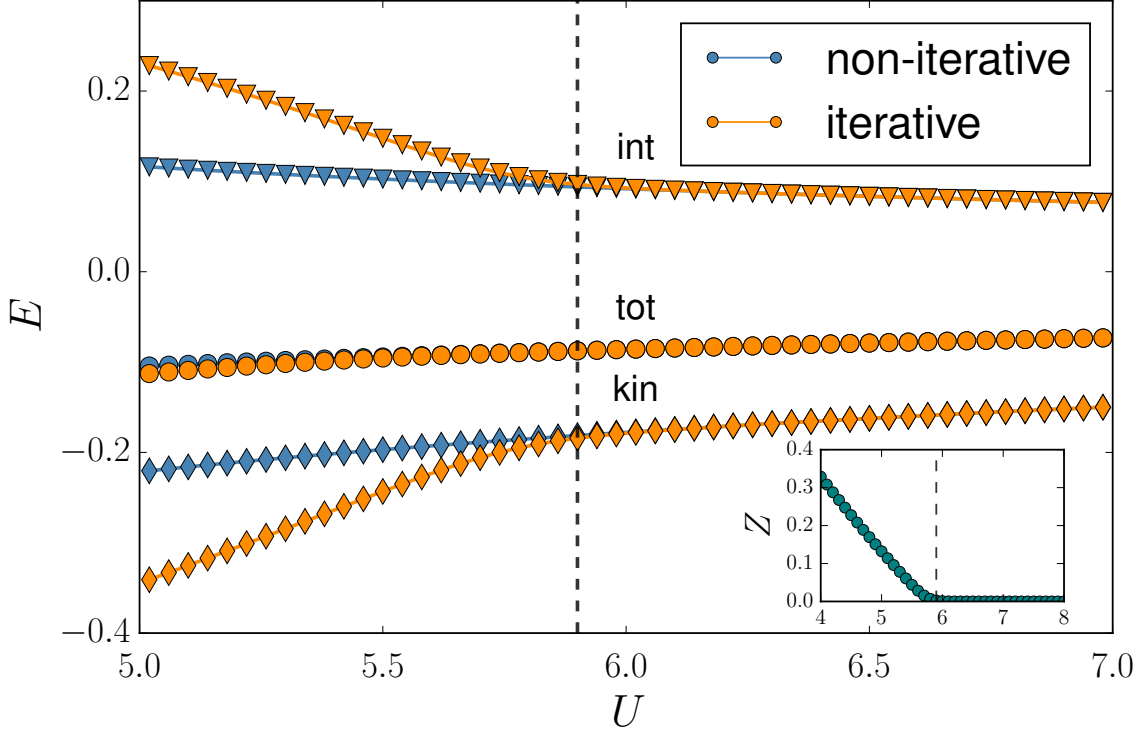


Figure 15: Comparison between the energies per site obtained with the iterative embedding scheme (*iterative*) and with the direct minimization of the impurity wavefunction (66) at $\phi = \pi/4$ (*non-iterative*): from top to bottom, local interaction energy (*int*), total energy (*tot*), and kinetic energy (*kin*), as a function of U . For each of them, the two methods coincide above U_c (dashed vertical line), where the system is in the paramagnetic Mott state. Inset: quasiparticle residue Z vs U , locating U_c .

4.2.1 The Mott transition in a magnetic field

A magnetic field that couples to the spin is the simplest perturbation that lifts the previously mentioned degeneracy in the Mott phase. It therefore provides a stringent test of the embedding scheme. We add to the Hamiltonian a Zeeman term,

$$H \rightarrow H - h \sum_i (n_{i\uparrow} - n_{i\downarrow}), \quad (68)$$

and work at fixed magnetic field $h = 0.01$. As mentioned in Chapter 3, an analogous problem was studied at fixed magnetization in [99] by direct minimization of the ghost-GA functional (28).

The effect of $h \neq 0$ on the Mott insulating phase can be anticipated from the zero-field results of the previous Section. In that Section, we found the energy $E(m)$ at fixed magnetization to be smooth and minimum at $m = 0$, see Fig. 14. As we switch on h , a Legendre transform maps the energy functional to

$$E(h) = \min_m (E(m) - hm). \quad (69)$$

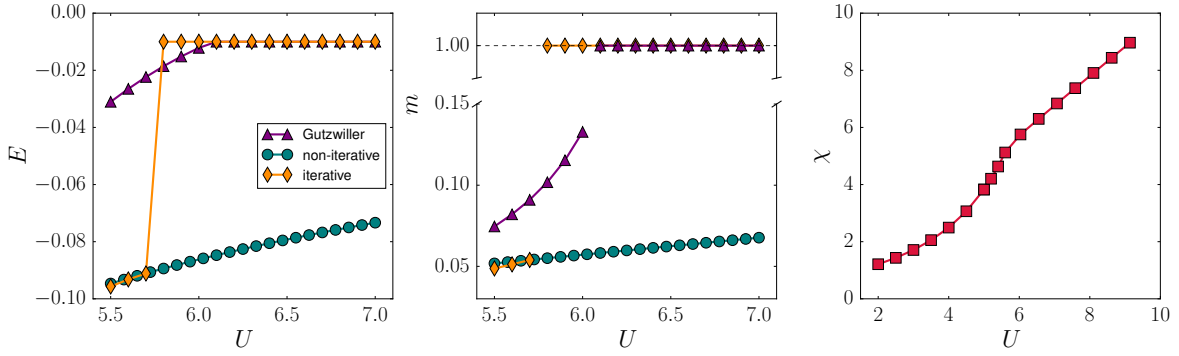


Figure 16: Ghost-GA results for the single-band Hubbard model in a magnetic field $h = 0.01$ across the Mott transition, comparing the iterative embedding scheme (*iterative*) with the direct minimization approach (*non-iterative*); the standard Gutzwiller approximation (*Gutzwiller*) is shown for reference. *Left panel:* energy per site E as a function of U . The iterative embedding energy displays an unphysical jump and, beyond it, collapses onto the standard GA energy, whereas direct minimization gives a smooth curve with lower energy. *Middle panel:* physical magnetization m as a function of U . Both the standard GA and the iterative embedding scheme reach a fully polarized $m = 1$ band insulator, while direct minimization remains only partially polarized, $m < 1$. *Right panel:* static zero-field spin susceptibility χ as a function of U , obtained from direct minimization in the Mott phase and from the embedding scheme in the metallic phase; χ stays finite and evolves continuously across the transition.

For any finite h , the minimum of $E(h)$ is displaced to a finite magnetization $\bar{m}(h)$, see the curve $E(h = 0.01)$ in Fig. 14. The system is therefore a partially polarized Mott insulator, with a finite magnetic susceptibility at zero field [15, 18, 99],

$$\chi = \partial_h \bar{m}|_{h \rightarrow 0} = \left(\partial_m^2 E(m) \right)_{\bar{m} \rightarrow 0}^{-1}. \quad (70)$$

We now examine how the embedding scheme (29) and the direct minimization of the ghost-GA functional (28) behave in this regime. We start from the embedding scheme. Naïvely, we could expect a finite field h to remove the primary difficulty encountered at zero field by lifting the ground state degeneracy. However, the resulting solution is unphysical. As shown in the left panel of Fig. 16, the embedding energy has a jump as U increases, which is physically incorrect. Beyond this jump, the solution collapses onto the conventional GA energy, also shown in the figure, and describes a fully polarized, $m = 1$, trivial band insulator with energy $E = -h$ per site, see the middle panel of Fig. 16. More details on the GA solution in a magnetic field are reported in Appendix B. A closely related instability has also been observed in zero-temperature DMFT, where the Mott insulating solution becomes fully polarized in an arbitrarily small magnetic field [122].

The direct minimization of the functional (28), using the wavefunction parametrization (66), does not suffer from this instability. The energy curve is smooth, with

no discontinuous jump, see the left panel of Fig. 16, and the corresponding Mott insulating solution remains only partially polarized with $m < 1$, see the middle panel of Fig. 16. Its variational energy is obviously lower than the unphysical fully polarized one.

Finally, the right panel of Fig. 16 shows the static zero-field spin susceptibility, computed from the direct-minimization solution in the Mott phase and using the embedding scheme in the metallic one. The susceptibility remains finite in the Mott phase and evolves continuously across the transition. This is a considerable improvement over the standard GA, which predicts a diverging susceptibility at the Mott transition, just as DMFT does [122] when one tries to compute the spin susceptibility from energetics instead of using the Bethe-Salpeter equation [4]. We remark that in standard Gutzwiller it is still possible to obtain a finite spin susceptibility in the Mott phase using an RPA approach [63], even though in that case the critical U_c is overestimated.

4.3 Antiferromagnetic phase

As discussed at the beginning of this Chapter, the difficulties encountered in iteratively solving the embedding problem can be traced back to the fact that the actual ground state of the half-filled Hubbard model on a bipartite lattice exhibits antiferromagnetic order, which is canted in the presence of a Zeeman field. Consequently, we anticipate that, when we allow for antiferromagnetism, the iterative method should converge effectively. This is precisely what we demonstrate in this Section comparing the results of the ghost-GA with DMFT.

Furthermore, one can readily adapt the aforementioned minimization scheme in the antiferromagnetic case by considering two distinct impurity wavefunctions for the two sublattices with opposite impurity magnetizations, m and $-m$, and determine the minimum with respect to m , as explained also in Section 3.4.3. In this case, we relax the constraint that the Hubbard bands are unpolarized so that $|\phi_n\rangle$, $n = 1, \dots, 4$, in (67) are replaced by

$$\begin{aligned}
 |\phi_1\rangle &= \frac{\sin \varphi}{\sqrt{2}} \left(|2, \downarrow, 0\rangle |\uparrow\rangle - |0, 2, \downarrow\rangle |\uparrow\rangle \right) - \frac{\cos \varphi}{\sqrt{2}} \left(|2, \uparrow, 0\rangle |\downarrow\rangle - |0, 2, \uparrow\rangle |\downarrow\rangle \right), \\
 |\phi_2\rangle &= \frac{\sin \varphi}{\sqrt{6}} \left(|\uparrow, \downarrow, \uparrow\rangle |\downarrow\rangle + |\uparrow, \uparrow, \downarrow\rangle |\downarrow\rangle - 2 |\uparrow, \downarrow, \downarrow\rangle |\uparrow\rangle \right) \\
 &\quad + \frac{\cos \varphi}{\sqrt{6}} \left(|\downarrow, \downarrow, \uparrow\rangle |\uparrow\rangle + |\downarrow, \uparrow, \downarrow\rangle |\uparrow\rangle - 2 |\downarrow, \uparrow, \uparrow\rangle |\downarrow\rangle \right), \\
 |\phi_3\rangle &= \frac{\sin \varphi}{\sqrt{2}} \left(|2, 0, \uparrow\rangle |\downarrow\rangle - |0, \uparrow, 2\rangle |\downarrow\rangle \right) + \frac{\cos \varphi}{\sqrt{2}} \left(|0, \downarrow, 2\rangle |\uparrow\rangle - |2, 0, \downarrow\rangle |\uparrow\rangle \right), \\
 |\phi_4\rangle &= -\cos \varphi |\uparrow, 0, 2\rangle |\downarrow\rangle + \sin \varphi |\downarrow, 0, 2\rangle |\uparrow\rangle,
 \end{aligned} \tag{71}$$

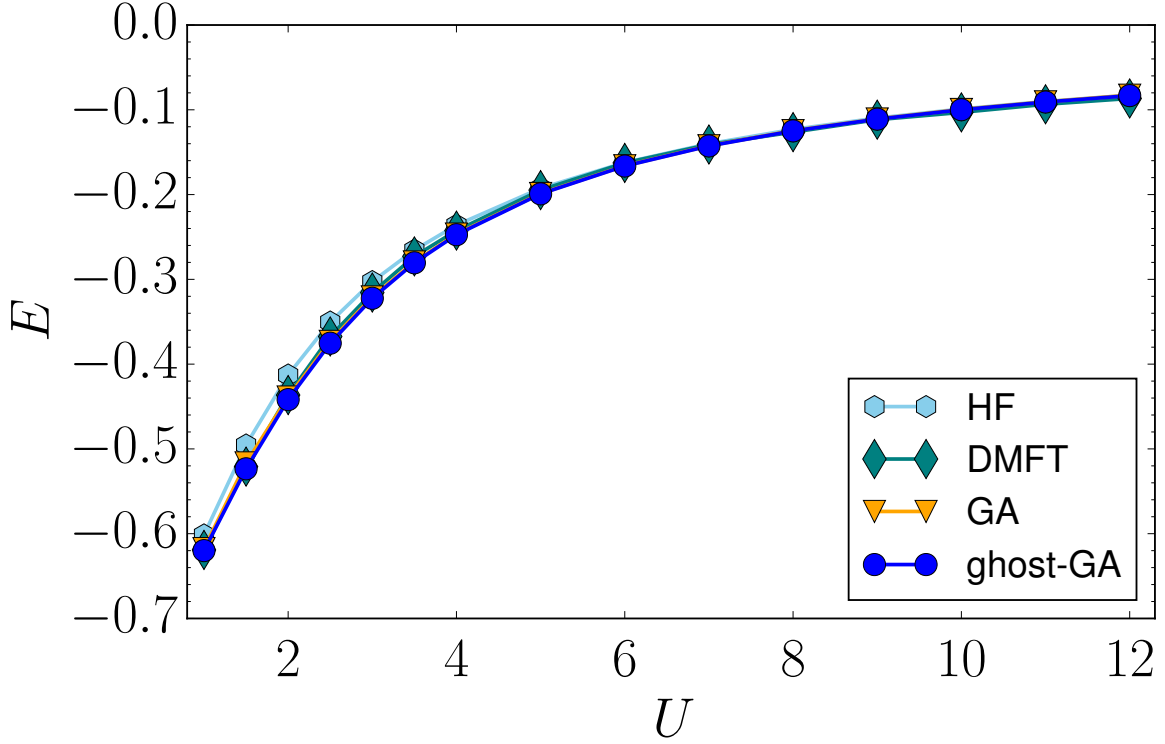


Figure 17: Total energy E versus U for the antiferromagnetic phase in the single-band Hubbard model, calculated using HF, DMFT, GA, and ghost-GA. At small U , the ghost-GA and DMFT energies are noticeably lower than those of HF and GA, whereas the differences become negligible at large U . DMFT data courtesy of Adriano Amaricci.

while $|\phi_0\rangle$ equals (65). The two wavefunctions corresponding to opposite magnetization are identified by $\varphi \in [0, \pi/4]$ and $\pi/2 - \varphi$. Details about the ghost-GA functional obtained from this impurity state are reported in Appendix D. The direct optimization using such impurity wavefunction, although now less accurate than the iterative embedding scheme, possesses the advantageous feature of describing states forced to have fixed and arbitrary order parameter, the staggered magnetization m . This is not feasible in the iterative schemes that directly provide the ground state value of m .

In Fig. 17 we compare the iterative ghost-GA results with the DMFT ones [123], which are obtained using exact diagonalization as impurity solver [124, 125]. The agreement is excellent, and both energies do not differ much from conventional GA as well as Hartree-Fock (HF), as noted in [19, 126]. In other words, the ground state properties in high dimensions are already well captured by HF, while dynamical ones may differ substantially [126, 127].

Having ascertained that the embedding scheme offers the same physical picture as DMFT, we proceed to study the antiferromagnetic phase through the variational minimization using the impurity wavefunction (66) with (65) and (71). The results of this method with those obtained by the embedding scheme are compared in Fig. 18.

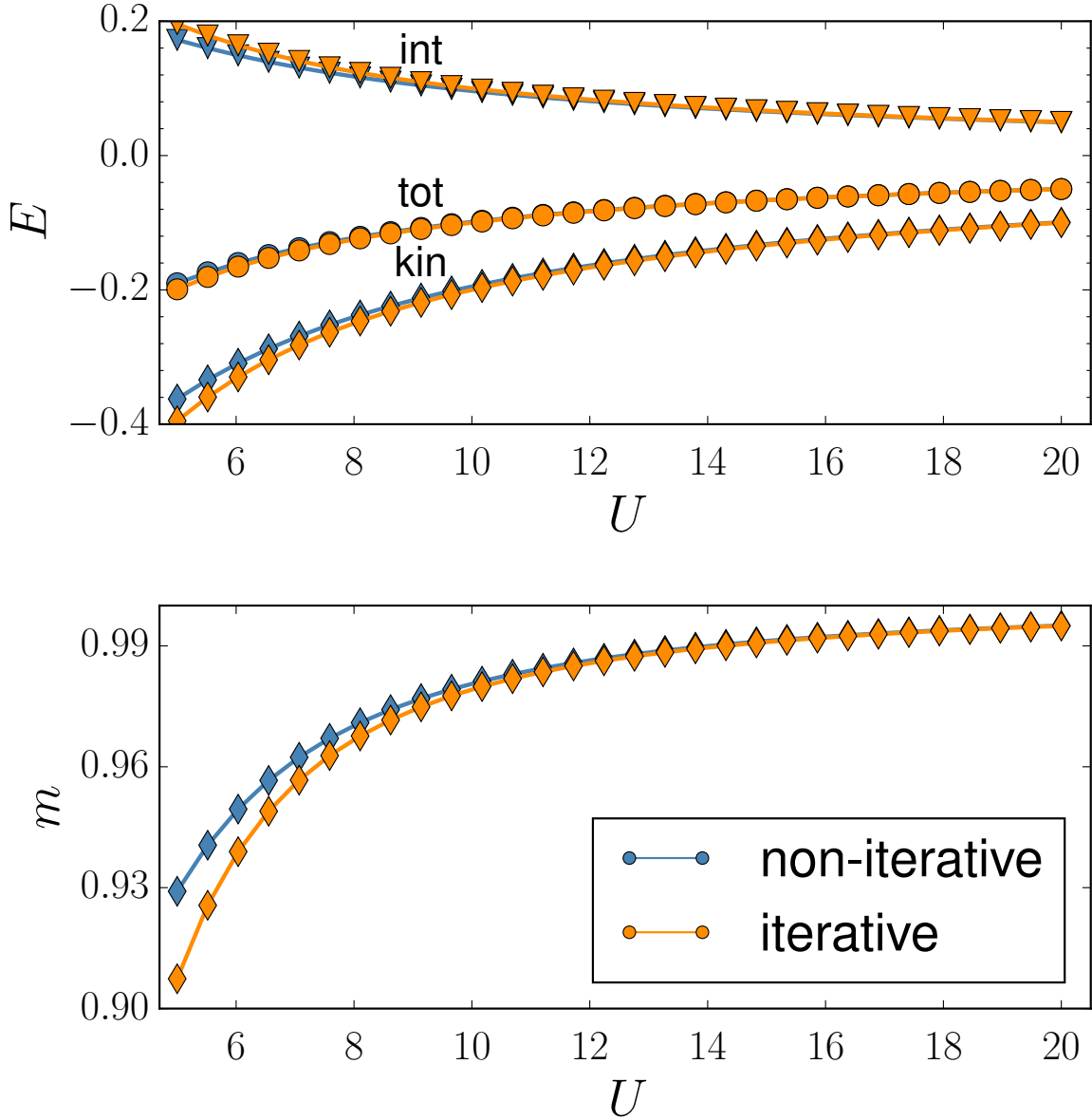


Figure 18: Comparison between energies, top panel, and magnetization, bottom panel, per site obtained through the iterative embedding scheme (*iterative*) and the direct minimization of the impurity wavefunction (71) (*non-iterative*). From top to bottom in the upper panel: local interaction energy (*int*), total energy (*tot*), and kinetic energy (*kin*), as a function of U .

We observe that the energy and magnetization of the embedding solution are lower than those obtained by the direct minimization, and become equal only at strong coupling.

The evidence that the DMFT, GA and ghost-GA values of m approach the maximum $m = 1$ value for large U , akin to HF, is a consequence of the inadequate description of spatial fluctuations of these methods that rely on the limit of infinite lattice coordination. In reality, the staggered magnetization saturates to a smaller value

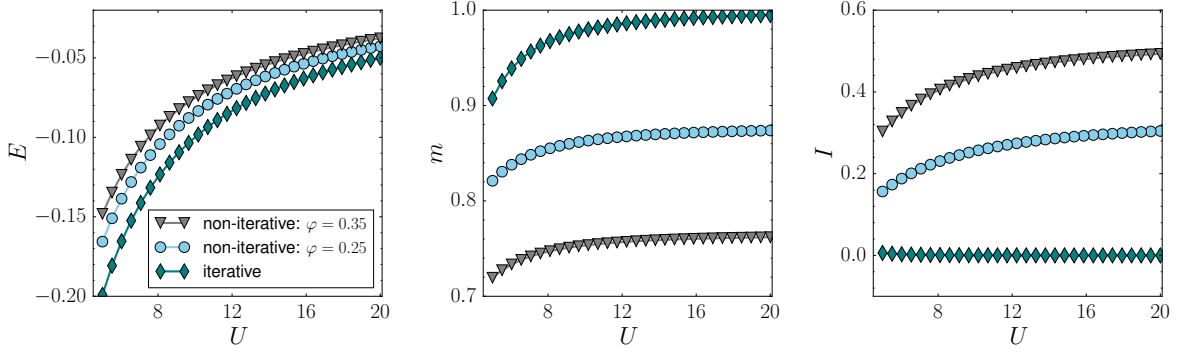


Figure 19: Comparison between the true ground state within the *iterative* embedding scheme and the *non-iterative* direct minimization using the impurity wavefunction (71) at fixed φ . From left to right: total energy per site, staggered magnetization m , and local mutual information I in units of $\ln 2$ as a function of U . Fixing φ makes it possible to stabilize more correlated states at the cost of a modest increase in variational energy.

as the lattice dimensionality decreases, thereby amplifying the effects of quantum fluctuations. A simple way to quantify the role of quantum fluctuations is the mutual information

$$I = S(\rho_{\uparrow}) + S(\rho_{\downarrow}) - S(\rho), \quad (72)$$

where ρ is the local reduced density matrix, ρ_{σ} is the spin-resolved one, and $S(\rho)$ the von Neumann entropy. This quantity is equivalent to the nonfreeness [128] and measures the distance of the state from a Gaussian one. It has been shown [128] that local embedding schemes, when allowed to break symmetry, generally reduce to a Hartree-Fock description in the strong-coupling limit with the mutual information I close to zero. The minimization of the ghost-GA functional (28) employing the impurity wavefunction (66) with components (65) and (71) presents a unique opportunity to access variationally states characterized by tunable staggered magnetization m , parametrized through the angle φ . In Fig. 19, we present the total energy per site, magnetization, and mutual information I of states optimized at fixed φ in comparison with the solution obtained within the embedding scheme. Notably, despite a relatively modest energy difference, the staggered magnetization m and, particularly, the mutual information, can exhibit substantial variations.

4.4 Conclusion

The ghost-Gutzwiller variational approach within the Gutzwiller approximation can be formulated in a quantum embedding scheme that comprises two self-consistently coupled variational wavefunctions. The first is the wavefunction of an impurity model, while the second is a Slater determinant ground state of a non-interacting periodic Hamiltonian with parameters that are non-linear functional of the impurity

wavefunction. The self-consistency condition establishes a connection between the local one-body density matrix of the Slater determinant and the reduced one-body density matrix of the bath in the impurity wavefunction. The most straightforward and efficient approach to solving the variational problem is by introducing a set of Lagrange multipliers that correspond to specific components of the reduced one-body density matrices. This allows the problem to be recast into two separate and self-consistently coupled eigenvalue problems, which can be readily solved iteratively.

We have demonstrated that this seemingly legitimate reformulation of the ghost-Gutzwiller variational problem may occasionally yield incorrect results. The flaw primarily arises when the physical Hamiltonian contains terms that split the degeneracy of the atomic limit pertinent to the Mott insulator. In the conventional Gutzwiller approximation, this circumstance leads to a first-order metal-insulator transition into a Mott phase where each site is frozen in the lowest-energy atomic configuration. In the ghost-Gutzwiller approximation, the Mott insulator remains unchanged, but the metal-insulator transition is accompanied by a finite jump in the variational energy, which is unphysical. We have shown that the correct results can be achieved by treating the complete impurity wavefunction as a variational object without requiring it to be the ground state of an Anderson impurity model. While this approach exhibits reduced efficiency compared to the iterative method, it presents significant advantages. Notably, it allows a straightforward enforcement of symmetries that may be broken in the actual ground state, thereby enabling the exploration of metastable states with intriguing properties, such as spin-charge fractionalization [15, 18, 24] or spin-liquid insulators. On the contrary, when we allow for symmetry breaking and the insulator is describable in mean-field, the iterative scheme is very efficient and provides sensible results.

5 | CONCLUSIONS

In this thesis we have shown that the ghost-Gutzwiller approximation can accurately describe a genuine paramagnetic Mott insulator: the auxiliary fermions that lose spectral weight at the Mott transition behave as physically meaningful, albeit spectroscopically invisible, quasiparticles, the *spinons*, which leave a measurable imprint whenever the insulator is perturbed, either by contact with a metallic reservoir or by an explicit symmetry-breaking field.

At the interface with a metal, spinons recombine with charge, thereby reacquiring spectral weight and forming heavy-fermion bands pinned at the chemical potential and confined within a surface layer whose depth diverges at the Mott transition. This phenomenon provides a natural explanation for the ambipolar in-gap states observed at the surface of the Ca_2RuO_4 correlated oxide.

In the bulk, the same zero-weight hidden quasiparticles are responsible for the genuinely paramagnetic response of the Mott insulator. A thorough analysis of a Mott insulator in a Zeeman spin-splitting field has shed light on certain subtleties within the ghost-Gutzwiller variational optimization. Specifically, we have discovered that the most efficient optimization method, which relies on the iterative solution of a quantum embedding problem, may fail in enforcing symmetries that are broken in the actual ground state. In such cases, alternative optimization strategies must be employed, which we illustrate through several examples.

Taken together, these results reframe the Mott gap not as a featureless void but as a reservoir of hidden low-energy degrees of freedom that can be converted into observable excitations by symmetry-breaking fields or by coupling to an external bath, and they position the ghost-Gutzwiller wavefunction as a computationally light yet physically faithful tool.

Several avenues for further research remain unexplored. Firstly, it would be worth extending the aforementioned alternative optimization strategies to more realistic multi-orbital models. Secondly, as briefly discussed in the Thesis, an intriguing issue lies in the residual gauge symmetry characterizing the ghost-Gutzwiller wavefunction of a symmetry-invariant Mott insulator, in contrast to the fully broken gauge symmetry observed in the metal phase. In a single-band model, we have identified this symmetry as a $\mathbb{Z}_2$ gauge symmetry, which is suggestive in light of the known classification of gapless spin-liquid insulators. It would be valuable to delve deeper into the role of gauge fixing exerted by the Gutzwiller constraints and the residual symmetries that are restored in the Mott insulator. This issue could

be addressed by incorporating quantum fluctuations through the time-dependent Gutzwiller approximation extended to include ghosts. This approach could also reveal the effective bandwidth of the concealed quasiparticles, which is not accessible in the straightforward ground state calculation and could be decisive in determining whether such quasiparticles possess physical significance and can be legitimately regarded as spinons. Finally, a further by-product of the time-dependent ghost-Gutzwiller approximation would consist in the calculation of dynamical response functions.

A

APPENDIX FOR THE CHAPTER: REVEALING SPINONS BY PROXIMITY EFFECT

A.1 Gutzwiller equations for the Metal-Mott interface

In this Appendix, we show the ghost-GA equations in the case of a metal-Mott insulator interface. We write the Gutzwiller constraints as:

$$\begin{aligned} \langle \phi(\ell) | \phi(\ell) \rangle &= 1, \\ \langle \phi(\ell) | d_{\ell\alpha\sigma} d_{\ell\alpha\sigma}^\dagger | \phi(\ell) \rangle &= \langle \Psi_* | d_{\ell r\beta\sigma}^\dagger d_{\ell r\alpha\sigma} | \Psi_* \rangle \equiv \Delta_{\alpha\sigma, \beta\sigma}(\ell), \end{aligned} \quad (\text{A.1})$$

where $\Delta_{\alpha\sigma, \beta\sigma}(\ell)$ define a matrix $\hat{\Delta}_\sigma(\ell)$. The iterative embedding equations, reported in 2.3.1, with the constraints written as in Eq. (A.1), can be written as:

$$\begin{aligned} \mathcal{H}_{qp} |\psi_*\rangle &= E_{qp} |\psi_*\rangle, \\ \left(\sqrt{\hat{\Delta}_\sigma(\ell)(1 - \hat{\Delta}(\ell)_\sigma)} \mathbf{V}_\sigma(\ell) \right)_\alpha &= \sum_{\mathbf{k}, \ell', \beta} R_{\beta\sigma}(\ell') \langle \Psi_* | d_{\ell\mathbf{k}\alpha\sigma}^\dagger d_{\ell'\mathbf{k}\beta\sigma} | \Psi_* \rangle t_{\ell\ell'}(\mathbf{k}), \\ \hat{\lambda}_\sigma(\ell) &= -\hat{\lambda}_\sigma^c(\ell) + \frac{\partial}{\partial \hat{\Delta}_\sigma(\ell)} \left(\mathbf{R}_\sigma(\ell) \cdot \sqrt{\hat{\Delta}_\sigma(\ell)(1 - \hat{\Delta}(\ell)_\sigma)} \mathbf{V}_\sigma(\ell) + H.c. \right), \\ \mathcal{H}_{imp}(\ell) | \phi(\ell) \rangle &= E_{imp}(\ell) | \phi(\ell) \rangle, \\ \langle \phi(\ell) | d_{\ell\alpha\sigma} d_{\ell\alpha\sigma}^\dagger | \phi(\ell) \rangle &= \langle \Psi_* | d_{\ell r\beta\sigma}^\dagger d_{\ell r\alpha\sigma} | \Psi_* \rangle = \Delta_{\alpha\sigma, \beta\sigma}(\ell), \\ R_{\alpha\sigma}(\ell) &= \sum_{\beta} \left(\sqrt{\hat{\Delta}_\sigma(\ell)(1 - \hat{\Delta}(\ell)_\sigma)} \right)_{\alpha, \beta}^{-1} \langle \phi(\ell) | c_{\ell\sigma}^\dagger d_{\ell\beta\sigma} | \phi(\ell) \rangle, \end{aligned} \quad (\text{A.2})$$

where

$$t_{\ell\ell'}(\mathbf{k}) = \delta_{\ell\ell'} \epsilon(\mathbf{k}) - t (\delta_{\ell', \ell+1} + \delta_{\ell', \ell-1}),$$

$\mathbf{R}_\sigma(\ell)$ and $\mathbf{V}_\sigma(\ell)$ are vectors with components $R_{\alpha\sigma}(\ell)$ and $V_{\alpha\sigma}(\ell)$, respectively, while $\hat{\lambda}_\sigma(\ell)$ and $\hat{\lambda}_\sigma^c(\ell)$ matrices with elements $\lambda_{\alpha\sigma, \beta\sigma}(\ell)$ and $\lambda_{\alpha\sigma, \beta\sigma}^c(\ell)$, respectively. The solution of Eq. (A.2) can be obtained self-consistently starting from a guess for $\mathbf{R}_\sigma(\ell)$ and $\hat{\lambda}_\sigma(\ell)$ and iterating the procedure till every equation is satisfied up to the desired accuracy.

A.2 Continuum description for the wetting critical behaviour

In the case of the conventional Gutzwiller approximation (GA), the Mott transition is first order but there is still a surface critical phenomenon, as shown in the main text. In this case, we can find a continuum description to extract the critical behaviour, as done in [97] at particle-hole (p-h) symmetry.

We write the impurity wavefunction as

$$|\phi(\ell)\rangle = \phi_0(\ell) |0, 2\rangle + \phi_2(\ell) |2, 0\rangle + \sum_{\sigma} \sigma \phi_{\sigma}(\ell) |\sigma, -\sigma\rangle ,$$

where $|\gamma_{imp}, \gamma_{bath}\rangle$ is a Fock state of the impurity plus the single bath level. Hereafter, we assume spin- $SU(2)$ symmetry, thus $\phi_{\sigma}(\ell) = \phi_1(\ell)$ independent of spin. For the standard Gutzwiller ansatz, we can write the energy functional per site as:

$$E = \frac{1}{N} \sum_{\ell} \left\{ \frac{U_{\ell}}{2} (\phi_0(\ell)^2 + \phi_2(\ell)^2) - \delta\mu \delta(\ell) \right\} + \frac{1}{N} \sum_{\ell} R_{\sigma}^2(\ell) \epsilon_{\ell} \\ + \frac{1}{N} \sum_{\ell} \sum_{p=\pm 1} R_{\sigma}(\ell) t_{\ell\ell+p} R_{\sigma}(\ell+p) ,$$

where N is the number of layers, each with $\mathcal{A}$ number of sites, and

$$\epsilon_{\ell} = \frac{1}{\mathcal{A}} \sum_{\mathbf{k}\sigma} \langle \Psi_* | c_{\ell\mathbf{k}\sigma}^{\dagger} \epsilon(\mathbf{k}) c_{\ell\mathbf{k}\sigma} | \Psi_* \rangle , \quad t_{\ell\ell'} = -\frac{t}{\mathcal{A}} \sum_{\mathbf{k}\sigma} \langle \Psi_* | c_{\ell\mathbf{k}\sigma}^{\dagger} c_{\ell'\mathbf{k}\sigma} | \Psi_* \rangle . \quad (\text{A.3})$$

The Gutzwiller constraints and the equation for $R_{\sigma}(\ell) = R(\ell)$ read:

$$1 = \phi_0(\ell)^2 + \phi_2(\ell)^2 + 2\phi_1(\ell)^2 , \\ n(\ell) = 1 - \delta(\ell) = 2\phi_2(\ell)^2 + 2\phi_1(\ell)^2 , \\ R(\ell)^2 = \frac{4}{1 - \delta(\ell)^2} \left(\phi_2(\ell) \phi_1(\ell) + \phi_0(\ell) \phi_1(\ell) \right)^2 .$$

We can choose to express the energy functional using $R(\ell)$ and the doping $\delta(\ell)$ as independent variables, in particular,

$$\phi_0(\ell)^2 + \phi_2(\ell)^2 \\ = \frac{1}{2} \left\{ 1 - \sqrt{(1 - R(\ell)^2)(1 - \delta(\ell)^2)} + \frac{\delta(\ell)^2}{1 - \sqrt{(1 - R(\ell)^2)(1 - \delta(\ell)^2)}} \right\} \quad (\text{A.4}) \\ \simeq \frac{1}{2} \left(1 - \sqrt{1 - R(\ell)^2} + \frac{\delta(\ell)^2}{2} \frac{1 + R(\ell)^2 + \sqrt{1 - R(\ell)^2}}{1 - \sqrt{1 - R(\ell)^2}} \right) ,$$

where the last equation is valid in the limit of small doping.

Near the critical point, the quantities in Eq. (A.3) do not depend appreciably on ℓ , $\epsilon_\ell \simeq -\epsilon_\parallel$ and $t_{\ell\ell\pm 1} \simeq -\epsilon_\perp/2$, so that, in the continuum limit $\ell \rightarrow x$, with continuous x , the energy functional reads

$$E = \int dx \left\{ \frac{U(x)}{2} [\phi_0(x)^2 + \phi_2(x)^2] - \epsilon R(x)^2 + \frac{\epsilon_\perp}{2} \left(\frac{\partial R(x)}{\partial x} \right)^2 - \delta\mu \delta(x) \right\}, \quad (\text{A.5})$$

where $\epsilon = \epsilon_\parallel + \epsilon_\perp$, and $\phi_0(x)^2 + \phi_2(x)^2$ is given by Eq. (A.4). Solving the Euler-Lagrange equations we can express $\delta(x)$ as a function of $R(x)$:

$$\delta(x) = \frac{4\delta\mu}{U(x)} \frac{1 - \sqrt{1 - R(x)^2}}{1 + R(x)^2 + \sqrt{1 - R(x)^2}}. \quad (\text{A.6})$$

The solution for $R(x)$ can be found deep in the Mott insulator, where $U(x) = U$ is constant and $R(x)$ and $\delta(x)$ are small. We find:

$$R(x) \simeq e^{-x/\xi}, \quad \delta(x) \simeq \text{sign}(\delta\mu) R(x)^2$$

with the correlation length given by

$$\frac{1}{\xi^2} = \frac{1}{\epsilon_\perp} \left(\frac{U}{4} - 2\epsilon - \frac{\delta\mu^2}{U} \right).$$

We note that ξ diverges at a critical $U = U_c$ which shifts to higher values at $\delta\mu \neq 0$, as expected.

B

GUTZWILLER RESULTS FOR THE HUBBARD MODEL IN A MAGNETIC FIELD

In this Appendix we present in more detail the standard Gutzwiller approximation (GA) results for the Hubbard model in a magnetic field, which are used in Chapter 4. We also give the argument that shows how the static magnetic susceptibility diverges at the Mott transition in GA.

In the conventional Gutzwiller wavefunction, one can parametrize the impurity wavefunction in terms of two angles θ and γ as:

$$|\phi\rangle = \cos\theta \left(\cos\gamma |\uparrow, \downarrow\rangle - \sin\gamma |\downarrow, \uparrow\rangle \right) + \frac{\sin\theta}{\sqrt{2}} \left(|0, 2\rangle + |2, 0\rangle \right). \quad (\text{B.1})$$

This results in a magnetization $m(\theta, \gamma) = \cos^2\theta \cos 2\gamma$ and a wavefunction renormalization:

$$R_{\uparrow}(\theta, \gamma) = R_{\downarrow}(\theta, \gamma) = \frac{\sin 2\theta}{\sqrt{1 - m(\theta, \gamma)^2}} \cos\left(\gamma - \frac{\pi}{4}\right). \quad (\text{B.2})$$

Furthermore, the average of the Hubbard repulsion term is given by:

$$\langle\phi| \frac{U}{2}(n-1)^2 |\phi\rangle = \frac{U}{2} \sin^2\theta. \quad (\text{B.3})$$

Including the Lagrange multipliers $\lambda_{\uparrow} = -\lambda_{\downarrow} = \lambda$ to fulfill the Gutzwiller constraints, the functional (28) to extremize is the following:

$$\begin{aligned} \mathcal{F}(\theta, \gamma, \lambda) = \int d\epsilon D(\epsilon) & \left((R(\theta, \gamma)^2 \epsilon - \lambda) f(R(\theta, \gamma)^2 \epsilon - \lambda) \right. \\ & \left. + (R(\theta, \gamma)^2 \epsilon + \lambda) f(R(\theta, \gamma)^2 \epsilon + \lambda) \right) \\ & + \frac{U}{2} \sin^2\theta + (\lambda - h)m(\theta, \gamma), \end{aligned}$$

where $f(x)$ is the Fermi distribution function at a sufficiently small temperature to make the integrand smooth without affecting the results. The results obtained with direct minimization are shown in Fig. 20, where we use the Bethe lattice density of states with $D = 2$ as in chapter 4. To conclude the appendix, we give a concise proof

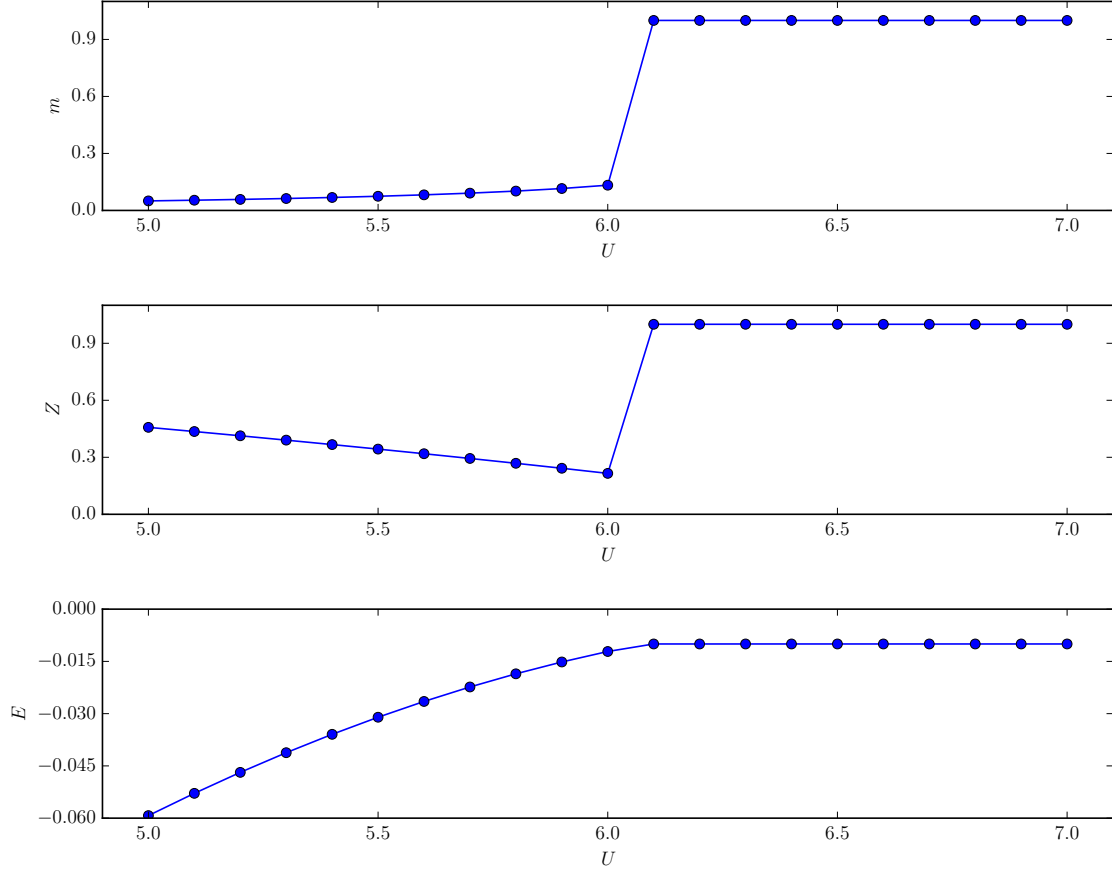


Figure 20: Results for the Hubbard model in a magnetic field for the conventional Gutzwiller wave function. We report the energy, the magnetization and the quasiparticle residue as a function of the interaction U for a fixed magnetic field $h = 0.01$. The results show a first-order transition between a correlated ferromagnetic metal and a fully polarized band insulator.

that the static magnetic susceptibility in the standard Gutzwiller approximation is infinite at the Mott transition. To do so, we use a constant density of states $D(\epsilon) = 1/(2D)$ for $|\epsilon| < D$ and zero otherwise to perform analytical calculations. The same results are obtained with a more general density of states. To calculate the magnetic susceptibility, we use the identity (70). Hence, we can calculate the energy at fixed magnetization m and then take the second derivative with respect to m . We start by calculating the kinetic energy at fixed magnetization m . We note that, in order to fix the number of particles with spin σ , we need to fulfil the following equations:

$$n_\sigma = \int_{-D}^{\mu_\sigma} d\epsilon D(\epsilon) , \quad (\text{B.4})$$

in the case of a constant density of states, this gives $\mu_\sigma = \sigma \frac{m}{D}$, with $\sigma = \pm 1$ for spin up and down, resulting in a kinetic energy at fixed magnetization

$$E_{kin}(m) = R^2 \sum_{\sigma} \int_{-D}^{\mu_{\sigma}} d\epsilon \epsilon D(\epsilon) = -R^2 \frac{D}{2} (1 - m^2) . \quad (\text{B.5})$$

In terms of the angles θ and $\varphi = \gamma - \pi/4$, we have an energy per site:

$$E(\theta, \varphi) = -\frac{D}{2} (1 - \cos^2 2\theta) \cos^2 \varphi + \frac{U}{2} \sin^2 \theta . \quad (\text{B.6})$$

We can rewrite the energy in terms of the magnetization m and the variable $x = \cos 2\theta$:

$$E(\theta, m) = -\frac{D}{4} (1 - x) \left(1 + x + \sqrt{(1 + x)^2 - 4m^2} \right) + \frac{U}{4} (1 - x) . \quad (\text{B.7})$$

For $m = 0$ the minimum is at $\bar{x} = \frac{U}{4D} \equiv u$ from which we can extract the value of the Mott transition $U_c = 4D$ without a magnetic field. We can now expand for small m around the minimum $\bar{x}$ by writing $x = \bar{x} + \delta x$ and expanding the energy to second order in δx and m :

$$E = -\frac{1}{2} (1 - u^2) + \frac{m^2}{2} \frac{1 - u}{1 + u} + \frac{\delta x^2}{2} - \frac{m^2}{(1 + u)^2} \delta x \quad (\text{B.8})$$

with minimum at $\delta x = \frac{m^2}{(1 + u)^2}$. Therefore, the energy at fixed magnetization $m \ll 1$ reads

$$E = -\frac{1}{2} (1 - u^2) + \frac{m^2}{2} \frac{1 - u}{1 + u} , \quad (\text{B.9})$$

from which we find $\chi = \frac{1 + m}{1 - m}$ that diverges at the Mott transition $u = 1$.

C

THE GHOST GUTZWILLER FUNCTIONAL FOR THE FERROMAGNETIC HUBBARD MODEL

We present here the functional to extremize for the ferromagnetic Hubbard model in a magnetic field within the ghost-Gutzwiller approximation and using the impurity state defined by the states in Eq. (67), hence the functional valid in the Mott phase. We start by computing the quasiparticle spectrum. We first evaluate the wavefunction renormalization matrix $\hat{R}$ through Eq. (25). We use the annihilation operators c_σ and $f_{a\sigma}$ for the physical and ghost orbitals, with $a = 1, 2$ for the lower and upper Hubbard band respectively. We start by computing the term $Q_{a\sigma}$ of equation (26) in terms of the impurity wavefunction parameters α_n and the angle φ :

$$\begin{aligned} Q_{1\uparrow} = Q_{2\downarrow} &= \frac{\sin \varphi}{2} \alpha_0 \alpha_1 + \left(\frac{1}{2\sqrt{3}} + \frac{\sin \varphi}{2\sqrt{6}} \right) \alpha_1 \alpha_2 \\ &\quad + \left(\frac{1}{2\sqrt{3}} + \frac{\cos \varphi}{2\sqrt{6}} \right) \alpha_2 \alpha_3 + \frac{\cos \varphi}{2} \alpha_3 \alpha_4, \\ Q_{1\downarrow} = Q_{2\uparrow} &= \frac{\cos \varphi}{2} \alpha_0 \alpha_1 + \left(\frac{1}{2\sqrt{3}} + \frac{\cos \varphi}{2\sqrt{6}} \right) \alpha_1 \alpha_2 \\ &\quad + \left(\frac{1}{2\sqrt{3}} + \frac{\sin \varphi}{2\sqrt{6}} \right) \alpha_2 \alpha_3 + \frac{\sin \varphi}{2} \alpha_3 \alpha_4. \end{aligned} \quad (\text{C.1})$$

Moreover, the diagonal entries of the local density matrix $\hat{\Delta}_\phi(\phi)$, i.e. the occupations of ghost orbitals for each spin, can be expressed as:

$$\begin{aligned} n_{1\uparrow} &:= \langle \psi | n_{1\uparrow} | \psi \rangle = \alpha_0^2 + \frac{3}{4} \alpha_1^2 + \frac{1}{2} \alpha_2^2 + \frac{1}{4} \alpha_3^2, \\ n_{1\downarrow} &:= \langle \psi | n_{1\downarrow} | \psi \rangle = \alpha_0^2 + \frac{3}{4} \alpha_1^2 + \frac{1}{2} \alpha_2^2 + \frac{1}{4} \alpha_3^2, \\ n_{2\uparrow} &:= \langle \psi | n_{2\uparrow} | \psi \rangle = \frac{1}{4} \alpha_1^2 + \frac{1}{2} \alpha_2^2 + \frac{3}{4} \alpha_3^2 + \alpha_4^2 \\ n_{2\downarrow} &:= \langle \psi | n_{2\downarrow} | \psi \rangle = \frac{1}{4} \alpha_1^2 + \frac{1}{2} \alpha_2^2 + \frac{3}{4} \alpha_3^2 + \alpha_4^2, \end{aligned}$$

For later convenience, we introduce the following quantity:

$$n_{1\uparrow} + n_{1\downarrow} - n_{2\uparrow} - n_{2\downarrow} = 2(\alpha_0^2 - \alpha_4^2) + (\alpha_1^2 - \alpha_3^2) := 2\Delta n. \quad (\text{C.2})$$

These occupations also determine $S_{a\sigma}^2 = n_{a\sigma}(1 - n_{a\sigma})$ entering $S(\hat{\Delta}_\phi)$ of Eq. (19), which turn out to be the same for both orbitals and both spins; and, for $a = 1, 2$,

$$S_{a\sigma}^2 := n_{a\uparrow}(1 - n_{a\uparrow}) = \frac{1}{4} \left(1 - (\Delta n)^2 \right) := S^2. \quad (\text{C.3})$$

Combining the factors $Q_{a\sigma}$ of Eq. (26) with S through the definition of $\hat{R}$ in Eq. (25), we obtain the wavefunction renormalization factor of each orbital and spin; therefore

$$\begin{aligned} R_{1\uparrow} &= \frac{Q_{1\uparrow}}{S} = R_{2\downarrow}, \\ R_{2\uparrow} &= \frac{Q_{2\uparrow}}{S} = R_{1\downarrow}. \end{aligned} \quad (\text{C.4})$$

We remark that since we constructed the impurity wavefunction to have a bath pinned at zero energy, the R component relative to that bath vanishes by construction. Finally, we report the two remaining impurity observables needed to evaluate the energy functional, Eq. (27), namely the physical magnetization and the operator entering the Hubbard interaction $(n - 1)^2$:

$$\begin{aligned} \langle \psi | n_\uparrow - n_\downarrow | \psi \rangle &= \cos 2\varphi \left(\alpha_0^2 - \frac{\alpha_2^2}{3} + \alpha_4^2 \right) := m, \\ \langle \psi | (n - 1)^2 | \psi \rangle &= \alpha_1^2 + \alpha_3^2. \end{aligned} \quad (\text{C.5})$$

We now build the lattice quasiparticle Hamiltonian $\mathcal{H}_{qp}$ of Eq. (31). It is convenient to trade the orbital-resolved renormalization factors $R_{1\sigma}$ and $R_{2\sigma}$ of Eq. (C.4) for their symmetric and antisymmetric combinations,

$$\begin{aligned} R_s &= \frac{R_{1\uparrow} + R_{2\uparrow}}{2} = \frac{R_{1\downarrow} + R_{2\downarrow}}{2}, \\ R_a &= \frac{R_{1\uparrow} - R_{2\uparrow}}{2} = -\frac{R_{1\downarrow} - R_{2\downarrow}}{2}, \end{aligned} \quad (\text{C.6})$$

and to parametrize the Lagrange multiplier matrix $\hat{\lambda}_\sigma$ in terms of the scalar parameters Δ , l and s :

$$\hat{\lambda}_\sigma = \Delta \hat{\tau}_3 + l \sigma \hat{\tau}_0 + s \sigma \hat{\tau}_1. \quad (\text{C.7})$$

Here, τ_i are the Pauli matrices, $\sigma = \pm 1$ for spin up and down, and $\hat{\lambda}_\sigma$ is a 2×2 matrix since the local potential for the decoupled bath is set to zero.

For a given dispersion $-\epsilon(\mathbf{k})$, the 2×2 quasiparticle Hamiltonian for up spins with lagrange multiplier then reads:

$$\mathcal{H}_\uparrow = -\epsilon(\mathbf{k}) \begin{pmatrix} (R_a + R_s)^2 & R_s^2 - R_a^2 \\ R_s^2 - R_a^2 & (R_s - R_a)^2 \end{pmatrix} - \begin{pmatrix} \Delta + l & s \\ s & l - \Delta \end{pmatrix} \quad (\text{C.8})$$

Diagonalizing $\mathcal{H}_\uparrow$ for each $\mathbf{k}$ gives the two spin-up quasiparticle bands:

$$\epsilon_{1,\uparrow}(\mathbf{k}) = -\sqrt{\epsilon(\mathbf{k}) (4\Delta R_a R_s - 2R_a^2 (s - \epsilon(\mathbf{k}) R_s^2) + \epsilon(\mathbf{k}) R_a^4 + \epsilon(\mathbf{k}) R_s^4 + 2s R_s^2) + \Delta^2 + s^2}$$

$$- \epsilon(\mathbf{k}) \left(R_a^2 + R_s^2 \right) + l, \quad (\text{C.9})$$

$$\begin{aligned} \epsilon_{2,\uparrow}(\mathbf{k}) = & \sqrt{\epsilon(\mathbf{k}) (4\Delta R_a R_s - 2R_a^2 (s - \epsilon(\mathbf{k}) R_s^2) + \epsilon(\mathbf{k}) R_a^4 + \epsilon(\mathbf{k}) R_s^4 + 2s R_s^2) + \Delta^2 + s^2} \\ & - \epsilon(\mathbf{k}) \left(R_a^2 + R_s^2 \right) - l \end{aligned} \quad (\text{C.10})$$

The Hamiltonian for spin-down electrons reads:

$$\mathcal{H}_\downarrow = -\epsilon(\mathbf{k}) \begin{pmatrix} (R_s - R_a)^2 & R_s^2 - R_a^2 \\ R_s^2 - R_a^2 & (R_a + R_s)^2 \end{pmatrix} - \begin{pmatrix} \Delta - l & -s \\ -s & -\Delta - l \end{pmatrix} \quad (\text{C.11})$$

Resulting in the two spin-down quasiparticle bands:

$$\begin{aligned} \epsilon_{1,\downarrow}(\mathbf{k}) = & -\sqrt{\epsilon(\mathbf{k}) (-4\Delta R_a R_s + 2R_a^2 (\epsilon(\mathbf{k}) R_s^2 + s) + \epsilon(\mathbf{k}) R_a^4 + \epsilon(\mathbf{k}) R_s^4 - 2s R_s^2) + \Delta^2 + s^2} \\ & - \epsilon(\mathbf{k}) \left(R_a^2 + R_s^2 \right) + l, \end{aligned} \quad (\text{C.12})$$

$$\begin{aligned} \epsilon_{2,\downarrow}(\mathbf{k}) = & \sqrt{\epsilon(\mathbf{k}) (-4\Delta R_a R_s + 2R_a^2 (\epsilon(\mathbf{k}) R_s^2 + s) + \epsilon(\mathbf{k}) R_a^4 + \epsilon(\mathbf{k}) R_s^4 - 2s R_s^2) + \Delta^2 + s^2} \\ & - \epsilon(\mathbf{k}) \left(R_a^2 + R_s^2 \right) + l \end{aligned} \quad (\text{C.13})$$

The quasiparticle Hamiltonian energy is obtained by filling the four quasiparticle bands $\epsilon_{n,\sigma}(\mathbf{k})$ up to the chemical potential. In practice, we numerically calculate the quasiparticle energy assuming a fictitious temperature β , with $\beta = 10^4$, so that the Fermi function effectively enforces zero-temperature filling while remaining smooth enough for the numerical integration:

$$E_{qp} = \int dx D(x) \sum_{n,\sigma} \epsilon_{n,\sigma}(x) f(\epsilon_{n,\sigma}(x)), \quad (\text{C.14})$$

with $f(x)$ the Fermi function and $D(x)$ the Bethe lattice density of states used in Chapter 4. It remains to specify the second, purely local term of Eq. (27), together with the Lagrange-multiplier term of Eq. (28) that depends on the impurity state, as the part depending on the Slater determinant has been absorbed in the quasiparticle Hamiltonian. Written in terms of the amplitudes $\alpha_0, \dots, \alpha_4$ and the angle φ , these read:

$$\langle \phi | \mathcal{H}_{loc} | \phi \rangle = -h \cos 2\varphi \left(\alpha_0^2 - \frac{1}{3} \alpha_2^2 + \alpha_4^2 \right) + \frac{U}{2} \left(\alpha_1^2 + \alpha_3^2 \right). \quad (\text{C.15})$$

The Lagrange multiplier term of Eq. (28) is

$$\mathcal{L} = -2\Delta \left(\alpha_0^2 + \frac{1}{2} \alpha_1^2 - \frac{1}{2} \alpha_3^2 + \alpha_4^2 \right) + E_\phi \left(1 - \sum_n \alpha_n^2 \right). \quad (\text{C.16})$$

Summing the quasiparticle energy E_{qp} , the local Hamiltonian $\langle \phi | \mathcal{H}_{loc} | \phi \rangle$ and the constraint term $\mathcal{L}$ reproduces the full functional as a function of φ , Δ , l , s and the various α_n . We numerically checked that the optimized Lagrange parameters l and s tend to zero at strong coupling, hence validating the assumption made in Sections 3.4.1 and 3.4.2.

D | THE GHOST GUTZWILLER FUNCTIONAL FOR THE AFM HUBBARD MODEL

We now present the calculations for the ghost-GA functional used for the Mott-AFM in Section 4.3. As anticipated in Chapter 2, capturing a two-sublattice AFM state requires promoting the variational matrix Λ , and hence the Lagrange multipliers and the wavefunction renormalization matrix $\hat{R}$, to be site-dependent, depending on the two sublattices A and B of the bipartite lattice; we use $(-1)^i$ to denote the sublattice sign. The local impurity wavefunction $|\psi\rangle$ is now that specified by the states in (71), which is still parametrized by the five amplitudes $\alpha_0, \dots, \alpha_4$ and by the angle φ . As for the ferromagnetic case, we start by evaluating the term $Q_{a\sigma}$ of equation (26), which now read

$$\begin{aligned} Q_{1\uparrow} = Q_{2\downarrow} &= \frac{1}{2\sqrt{2}} (1 - \cos 2\varphi) \alpha_0 \alpha_1 + \frac{1}{4\sqrt{3}} (2 + \sin 2\varphi - 2 \cos 2\varphi) \alpha_1 \alpha_2 \\ &\quad + \frac{1}{4\sqrt{3}} (1 + 2 \sin 2\varphi + \cos 2\varphi) \alpha_2 \alpha_3 + \frac{1}{2\sqrt{2}} \sin 2\varphi \alpha_3 \alpha_4, \\ Q_{2\uparrow} = Q_{1\downarrow} &= \frac{1}{2\sqrt{2}} (1 + \cos 2\varphi) \alpha_0 \alpha_1 + \frac{1}{4\sqrt{3}} (2 + \sin 2\varphi + 2 \cos 2\varphi) \alpha_1 \alpha_2 \\ &\quad + \frac{1}{4\sqrt{3}} (1 + 2 \sin 2\varphi - \cos 2\varphi) \alpha_2 \alpha_3 + \frac{1}{2\sqrt{2}} \sin 2\varphi \alpha_3 \alpha_4. \end{aligned}$$

Moreover, the local occupations of the ghost orbitals for each spin follow again from the amplitudes $\alpha_0, \dots, \alpha_4$:

$$\begin{aligned} n_{1\uparrow} &= \alpha_0^2 + \frac{3}{4} \alpha_1^2 + \frac{1}{4} \cos 2\varphi \alpha_1^2 + \frac{1}{2} \alpha_2^2 + \frac{1}{3} \cos 2\varphi \alpha_2^2 + \frac{1}{4} \alpha_3^2 - \frac{1}{4} \cos 2\varphi \alpha_3^2, \\ n_{1\downarrow} &= \alpha_0^2 + \frac{3}{4} \alpha_1^2 - \frac{1}{4} \cos 2\varphi \alpha_1^2 + \frac{1}{2} \alpha_2^2 - \frac{1}{3} \cos 2\varphi \alpha_2^2 + \frac{1}{4} \alpha_3^2 + \frac{1}{4} \cos 2\varphi \alpha_3^2, \\ n_{2\uparrow} &= \frac{1}{4} \alpha_1^2 + \frac{1}{4} \cos 2\varphi \alpha_1^2 + \frac{1}{2} \alpha_2^2 + \frac{1}{3} \cos 2\varphi \alpha_2^2 + \frac{3}{4} \alpha_3^2 - \frac{1}{4} \cos 2\varphi \alpha_3^2 + \alpha_4^2, \\ n_{2\downarrow} &= \frac{1}{4} \alpha_1^2 - \frac{1}{4} \cos 2\varphi \alpha_1^2 + \frac{1}{2} \alpha_2^2 - \frac{1}{3} \cos 2\varphi \alpha_2^2 + \frac{3}{4} \alpha_3^2 + \frac{1}{4} \cos 2\varphi \alpha_3^2 + \alpha_4^2, \end{aligned}$$

To simplify the expression for the local density matrix, we introduce the following quantities:

$$\begin{aligned} n_{1\uparrow} + n_{1\downarrow} - n_{2\uparrow} - n_{2\downarrow} &= 2(\alpha_0^2 - \alpha_4^2) + (\alpha_1^2 - \alpha_3^2) = 2\Delta n, \\ n_{1\uparrow} - n_{1\downarrow} &= n_{2\uparrow} - n_{2\downarrow} = \frac{1}{2} \cos 2\varphi \alpha_1^2 + \frac{2}{3} \cos 2\varphi \alpha_2^2 - \frac{1}{2} \cos 2\varphi \alpha_3^2 = \Delta m, \end{aligned}$$

In terms of these quantities, $S_{a\sigma}^2 = n_{a\sigma}(1 - n_{a\sigma})$ in equation (19) read

$$\begin{aligned} S_{1\uparrow}^2 &= n_{1\uparrow}(1 - n_{1\uparrow}) = \frac{1}{4} \left(1 - (\Delta n + \Delta m)\right)^2 = S_{2\downarrow}^2, \\ S_{2\uparrow}^2 &= n_{1\uparrow}(1 - n_{1\uparrow}) = \frac{1}{4} \left(1 - (\Delta n - \Delta m)\right)^2 = S_{1\downarrow}^2, \end{aligned}$$

From which we can compute the wavefunction renormalization factors $R_{a\sigma}$ of each orbital and spin

$$R_{1\uparrow} = R_{2\downarrow}, \quad R_{2\uparrow} = R_{1\downarrow}.$$

We start the construction of the functional by evaluating the kinetic part of the quasiparticle Hamiltonian $\mathcal{H}_{qp}$ of Eq. (31), that for the single band Hubbard model reads

$$T = - \sum_{\langle ij \rangle} \sum_{a,b=1}^2 \sum_{\sigma} R_{ia\sigma} R_{jb\sigma} \left(f_{ia\sigma}^\dagger f_{jb\sigma} + f_{jb\sigma}^\dagger f_{ia\sigma} \right).$$

It is useful, in order to make connection with the results presented in paragraph 3.4.3, to decompose the quasiparticle renormalization factors $R_{ia\sigma}$ in terms of a uniform and a staggered component:

$$\begin{aligned} R_{i1\uparrow} &= R_{i2\downarrow} = R \cos \phi + (-1)^i R \sin \phi, \\ R_{i1\downarrow} &= R_{i2\uparrow} = R \cos \phi - (-1)^i R \sin \phi. \end{aligned}$$

where, the angle ϕ in the previous equations, in the case of the most general impurity state, it is a function of φ and the amplitudes α_n . To evaluate the hopping term T , we need the products of renormalization factors on neighboring sites i and j . It follows that, for i and j nearest neighbors,

$$R_{ia\sigma} R_{ja\sigma} = R^2 \cos 2\phi, \quad a = 1, 2, \quad \sigma = \uparrow, \downarrow,$$

i.e. the intra-orbital hopping amplitude is uniform across the lattice, while the inter-orbital one picks up a staggered contribution:

$$\begin{aligned} R_{i1\uparrow} R_{j2\uparrow} &= R_{i2\downarrow} R_{j1\downarrow} = \left(R \cos \phi + (-1)^i R \sin \phi \right)^2 \\ &= R^2 + (-1)^i R^2 \sin 2\phi, \\ R_{i1\downarrow} R_{j2\downarrow} &= R_{i2\uparrow} R_{j1\uparrow} = \left(R \cos \phi - (-1)^i R \sin \phi \right)^2 \\ &= R^2 - (-1)^i R^2 \sin 2\phi. \end{aligned}$$

Collecting all the contributions, the hopping is therefore

$$\begin{aligned}
T = & -R^2 \cos 2\phi \sum_{\langle ij \rangle} \sum_{a=1}^2 \sum_{\sigma} \left(f_{ia\sigma}^\dagger f_{ja\sigma} + f_{ja\sigma}^\dagger f_{ia\sigma} \right) \\
& - R^2 \sum_{\langle ij \rangle} \sum_{a \neq b} \sum_{\sigma} \left(f_{ia\sigma}^\dagger f_{jb\sigma} + f_{jb\sigma}^\dagger f_{ia\sigma} \right) \\
& - R^2 \sin 2\phi \sum_{\langle ij \rangle} (-1)^i \sum_{\sigma} \sigma \left(f_{i1\sigma}^\dagger f_{j2\sigma} - f_{i2\sigma}^\dagger f_{j1\sigma} + f_{j2\sigma}^\dagger f_{i1\sigma} - f_{j1\sigma}^\dagger f_{i2\sigma} \right),
\end{aligned}$$

Fourier transforming the fermionic operators in momentum space, we obtain

$$\begin{aligned}
T = & -R^2 \cos 2\phi \sum_{\mathbf{k}\sigma} \sum_{a=1}^2 \epsilon(\mathbf{k}) f_{\mathbf{k}a\sigma}^\dagger f_{\mathbf{k}a\sigma} - R^2 \sum_{\mathbf{k}\sigma} \sum_{a \neq b} \epsilon(\mathbf{k}) f_{\mathbf{k}a\sigma}^\dagger f_{\mathbf{k}b\sigma} \\
& - R^2 \sin 2\phi \sum_{\mathbf{k}\sigma} \sigma \epsilon(\mathbf{k}) \left(f_{\mathbf{k}2\sigma}^\dagger f_{\mathbf{k}+\mathbf{Q}1\sigma} - f_{\mathbf{k}1\sigma}^\dagger f_{\mathbf{k}+\mathbf{Q}2\sigma} \right),
\end{aligned}$$

where $-\epsilon(\mathbf{k})$ is the lattice dispersion and $\mathbf{Q} = (\pi, \dots, \pi)$ is the AFM ordering wavevector, which connects the two sublattices and couples $\mathbf{k}$ to $\mathbf{k} + \mathbf{Q}$ in the staggered term above, the length of the $\mathbf{Q}$ vector is the same as the dimension of the lattice. Following the standard zone-folding procedure, we restrict momenta to the reduced Brillouin zone (RBZ) and relabel the operators at $\mathbf{k}$ and $\mathbf{k} + \mathbf{Q}$ as belonging, respectively, to the f and d flavor: for $\mathbf{k} \in \text{RBZ}$, we define

$$f_{\mathbf{k}a\sigma} \equiv f_{\mathbf{k}a\sigma}, \quad f_{\mathbf{k}+\mathbf{Q}a\sigma} \equiv d_{\mathbf{k}a\sigma},$$

and define the spinor

$$\Psi_{\mathbf{k}\sigma} = \begin{pmatrix} f_{\mathbf{k}1\sigma} \\ f_{\mathbf{k}2\sigma} \\ d_{\mathbf{k}1\sigma} \\ d_{\mathbf{k}2\sigma} \end{pmatrix}.$$

With these notations, the hopping term for each spin T_σ becomes a 4×4 matrix acting on $\Psi_{\mathbf{k}\sigma}$ for each $\mathbf{k}$ in the reduced Brillouin zone,

$$T_\sigma(\mathbf{k}) = -R^2 \epsilon(\mathbf{k}) \begin{pmatrix} \cos 2\phi & 1 & 0 & -\sigma \sin 2\phi \\ 1 & \cos 2\phi & \sigma \sin 2\phi & 0 \\ 0 & \sigma \sin 2\phi & -\cos 2\phi & -1 \\ -\sigma \sin 2\phi & 0 & -1 & -\cos 2\phi \end{pmatrix}.$$

Introducing the Pauli matrices σ_α and τ_α , $\alpha = 0, 1, 2, 3$, the former acting in the 1-2 space and the latter in the c - d one, we can parametrize the lagrange multiplier matrix $\hat{\lambda}$ in terms of the scalar parameters μ , λ_{01} , λ_{11} as:

$$\hat{\lambda}_\sigma = -\mu \hat{\sigma}_3 \otimes \hat{\tau}_0 - \sigma \lambda_{01} \hat{\sigma}_0 \otimes \hat{\tau}_1 - \sigma \lambda_{11} \hat{\sigma}_1 \otimes \hat{\tau}_1. \quad (\text{D.1})$$

Hence we have a quasiparticle Hamiltonian for each spin σ that reads

$$H_\sigma(\mathbf{k}) = -\mu \hat{\sigma}_3 \otimes \hat{\tau}_0 - \sigma \lambda_{01} \hat{\sigma}_0 \otimes \hat{\tau}_1 - \sigma \lambda_{11} \hat{\sigma}_1 \otimes \hat{\tau}_1 - R^2 \epsilon(\mathbf{k}) \cos 2\phi \hat{\sigma}_0 \otimes \hat{\tau}_3 \\ - R^2 \epsilon(\mathbf{k}) \hat{\sigma}_1 \otimes \hat{\tau}_3 - \sigma R^2 \epsilon(\mathbf{k}) \sin 2\phi \hat{\sigma}_2 \otimes \hat{\tau}_2, \quad (\text{D.2})$$

The last Hamiltonian can be readily diagonalized by introducing the two functions

$$E_1(\mathbf{k}) = \sqrt{(\mu R^2 \epsilon(\mathbf{k}) \cos 2\phi - \lambda_{11} R^2 \epsilon(\mathbf{k}) \sin 2\phi)^2 + (R^4 \epsilon(\mathbf{k})^2 \sin 2\phi + \mu \lambda_{01})^2}. \quad (\text{D.3})$$

and

$$E_2(\mathbf{k}) = \sqrt{(R^4 \epsilon(\mathbf{k})^2 \cos 2\phi + \lambda_{01} \lambda_{11})^2 + E_1(\mathbf{k})^2}. \quad (\text{D.4})$$

in terms of which we have the following eigenvalues of $H_\sigma(\mathbf{k})$:

$$\epsilon_1(\mathbf{k}) = -\sqrt{\mu^2 + 2 R^4 \epsilon(\mathbf{k})^2 + \lambda_{01}^2 + \lambda_{11}^2 - 2 E_2(\mathbf{k})}, \\ \epsilon_2(\mathbf{k}) = -\sqrt{\mu^2 + 2 R^4 \epsilon(\mathbf{k})^2 + \lambda_{01}^2 + \lambda_{11}^2 + 2 E_2(\mathbf{k})}, \quad (\text{D.5}) \\ \epsilon_3 = -\epsilon_1, \\ \epsilon_4 = -\epsilon_2.$$

In conclusion, the ground state energy of the quasiparticle Hamiltonian is simply

$$E_{qp} = -\frac{2}{V} \sum_{\mathbf{k} \in \text{RBZ}} (\epsilon_1(\mathbf{k}) + \epsilon_2(\mathbf{k})). \quad (\text{D.6})$$

The last terms needed to evaluate the ghost Gutzwiller functional for the variational minimization are the Hubbard repulsion term and the Lagrange multiplier term. The average of the Hubbard repulsion term is given by:

$$\langle \phi | \mathcal{H}_{loc} | \phi \rangle = \frac{U}{2} (\alpha_1^2 + \alpha_3^2), \quad (\text{D.7})$$

while the Lagrange multiplier part is

$$\mathcal{L} = -2\mu \Delta n - 2\lambda_{01} \Delta m + E_\phi \left(1 - \sum_n \alpha_n^2\right). \quad (\text{D.8})$$

As for the ferromagnetic case, summing the quasiparticle energy E_{qp} , the local Hamiltonian $\langle \phi | \mathcal{H}_{loc} | \phi \rangle$ and the constraint term $\mathcal{L}$ reproduces the full functional for which we find the saddle point as a function of ϕ , μ , λ_{01} , λ_{11} and the various α_n .

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