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

The Many Guises of Quasiparticles in Correlated Electron Systems

PhD thesis

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Abstract

Many strongly correlated electron systems fall outside the conventional quasiparticle paradigm. Their low-energy fermionic excitations need not be adiabatically connected to the bare electrons or appear as poles of the physical electron single-particle Green's function. This thesis investigates to what extent an effective quasiparticle description can nevertheless survive, and which emergent degrees of freedom provide the appropriate low-energy structure.

First, the interaction-driven evolution from a quantum spin Hall insulator to a Mott insulator is studied using the dynamical cluster approximation. Dispersive zeros of the single-particle Green's function emerge near the Mott transition and retain a nontrivial topological character. When symmetry breaking is allowed, a nontopological excitonic insulator is found to intrude between quantum spin Hall and Mott insulators. Encoding both poles and zeros within a low-energy quasiparticle Hamiltonian provides a continuous one-body description of the three phases. On the Mott side, its gap evolution supports interpreting the soft excitonic mode as a bound state of quasiparticle and quasihole excitations tied to the Green's function zeros, rather than to the widely separated Hubbard bands.

Second, the intrinsic anomalous Hall conductivity of a topological metal is analyzed within a multiband extension of Landau Fermi-liquid theory. Residual interactions among quasiparticles at the Fermi surface dress the dynamic current vertex and generate corrections to the Berry-curvature contribution obtained from the quasiparticle bands alone. Our result supports recent claims that the correct expressions for topological observables include vertex corrections besides the topological invariants built just upon the Green's function. It also demonstrates that such corrections are naturally accounted for by Landau Fermi-liquid theory.

Extracting the relevant ingredients for an effective description of material-relevant correlated systems requires computational tools that remain reliable at low temperatures. To this end, a deterministic strong-coupling impurity solver for dynamical mean-field theory is discussed. By providing static, dynamical, and thermodynamic observables without stochastic sampling, it offers a promising route toward multiorbital and spin-orbit coupled problems where conventional Monte Carlo methods currently struggle.

Finally, the auxiliary quasiparticle framework underlying the ghost-Gutzwiller Ansatz is investigated. On a model for correlated quantum spin Hall insulators, we show that the topology of the interacting state is encoded in the auxiliary one-body Hamiltonian. The resulting band-structure reveals topological Hubbard bands whose topological character can be tuned through a finite magnetization. When applied to the single-band t - J model, the same framework yields a fractionalized Fermi liquid (FL^{*}). In this phase, dispersive neutral spinons, with vanishing physical-electron spectral weight, coexist with conventional quasiparticles forming a small hole-like Fermi surface, thus violating Luttinger's theorem. The corresponding temperature-doping phase diagram contains a low-doping FL^{*}, a d -wave superconducting dome, and an overdoped conventional Fermi liquid, thereby reproducing key qualitative features of cuprate phenomenology.

Publications

The topics discussed in this thesis are covered in the following works:

1. **I. Pasqua**, A. Blason, and M. Fabrizio, *Exciton condensation driven by bound states of Green's function zeros*, [Phys. Rev. B **110**, 125144 \(2024\)](#). [Chapter 1]
2. **I. Pasqua** and M. Fabrizio, *Fermi-liquid corrections to the intrinsic anomalous Hall conductivity of topological metals*, [SciPost Phys. **19**, 014 \(2025\)](#). [Chapter 2]
3. **I. Pasqua**, J. Kaye, and A. Georges, *Static and dynamical properties of a strong-coupling impurity solver for dynamical mean-field theory*, in preparation (2026). [Chapter 3]
4. **I. Pasqua**, A. M. Tagliente, G. Bellomia, B. Monserrat, M. Fabrizio, and C. Mejuto Zaera, *Band-structure picture for topology in strongly correlated systems with the ghost Gutzwiller ansatz*, [Phys. Rev. B **113**, 155133 \(2026\)](#). [Chapter 4]
5. **I. Pasqua**, C. Mejuto Zaera, and M. Fabrizio, *Fractionalized Fermi liquids with the ghost-Gutzwiller Ansatz*, [arXiv:2607.12410](#) (2026). [Chapter 5]

During my PhD, I also contributed to the following publications not discussed in this thesis:

1. S. Del Puppo, P. Biasin, A. Sala, P. Mantegazza, **I. Pasqua**, E. Ghidorsi, M. Caporali, A. Resta, A. Coati, F. Genuzio, T. O. Mentec, A. Locatelli, G. Comelli, C. Africh, E. Vesselli, M. Peressi, and A. Verdini, *Blue phosphorene on Au(111): theoretical, spectroscopic and diffraction analysis reveal the role of single Au adatoms*, [Nanoscale Adv. **6**, 3582 \(2024\)](#).
2. A. Blason, **I. Pasqua**, M. Ferrero, and M. Fabrizio, *Luttinger surface dominance and Fermi liquid behaviour of topological Kondo insulators SmB_6 and YbB_{12}* , [Phys. Rev. B **110**, 235115 \(2024\)](#).
3. **I. Pasqua**, G. Staffieri, and M. Fabrizio, *How chiral vibrations drive molecular rotation*, [Phys. Rev. B **112**, 094303 \(2025\)](#).
4. A. M. Tagliente*, **I. Pasqua***, and M. Fabrizio, *Direct minimization versus iterative embedding in the ghost-Gutzwiller method: a comparative study of magnetism in Mott insulators*, [arXiv:2607.27156](#) (2026).

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Contents

Introduction	1
1 Exciton condensation driven by bound states of Green’s function zeros	13
1.1 A simple model for correlated quantum spin Hall insulators	15
1.2 Exciton bound states softening into an excitonic insulator	19
1.3 The Green’s function framework: poles, zeros, and topology	21
1.4 The symmetric QSHI–MI transition	25
1.5 The excitonic instability	32
1.6 Conclusions	37
2 Fermi liquid corrections to the intrinsic anomalous Hall conductivity of topological metals	39
2.1 Hall conductivity within Landau’s Fermi liquid theory	40
2.2 An explicit toy model calculation	48
2.3 Conclusions	53
3 Static and dynamical properties of a strong-coupling impurity solver for dynamical mean-field theory	55
3.1 Strong-coupling expansion and pseudoparticle representation	57
3.2 Computing physical quantities	60
3.3 Results on the single-band Hubbard model	66
3.4 Conclusions	77
4 Topology, correlations and magnetism with the ghost-Gutzwiller Ansatz	79
4.1 Overview of the ghost-Gutzwiller formalism	81
4.2 Topology within the ghost-Gutzwiller formalism	85
4.3 Benchmarks and quasiparticle perspective	90
4.4 OBC calculations and edge states in the quasiparticle Hamiltonian . . .	93
4.5 Topology of the Hubbard bands and their interplay with magnetism . .	96
4.6 Conclusions	102
5 Fractionalized Fermi liquids with the ghost-Gutzwiller Ansatz	105
5.1 Extension to non-local spin-spin interactions	107
5.2 Model and variational wavefunction	111

5.3	Variational Ansatz at finite temperature	117
5.4	Temperature–doping phase diagram	122
5.5	Conclusions	124
A	Mean-field decoupling of the spin-spin exchange on a d-wave BCS state	126
Conclusions		129
Bibliography		131

Introduction

Some of the most striking phenomena in condensed matter physics arise from the collective behavior of systems with many interacting degrees of freedom. At low energies, these systems are often governed by emergent excitations that bear little resemblance to their microscopic constituents and whose properties cannot be understood by following the underlying particles individually. A central challenge is therefore to identify the appropriate emergent degrees of freedom and to develop theoretical descriptions that capture their dynamics. This task may require entirely new conceptual frameworks as well as analytical and computational tools, but the effort pays off by revealing physics that is both unexpected and richer than one could have envisioned, even with the most fervent human imagination.

Effective one-body theories provide a powerful realization of this strategy. By recasting the collective behavior of an interacting many-body system in terms of suitably defined and weakly interacting quasiparticles, they replace a problem whose complexity grows exponentially with system size with a tractable theoretical framework, while retaining the essential physics. At the same time, they offer an intuitive picture of the mechanisms underlying remarkable phenomena. Historically, the first identified quasiparticles were the phonons, which describe at low-temperature the lattice vibrational modes in terms of non-interacting bosons plus a residual weak-interaction that accounts for anharmonicity [1, 2]. However, over the years, these attempts have transcended lattice vibrations, encompassing a wide range of phenomena from the Fermi-liquid properties of metals [3, 4] to the topological nature of the integer quantum Hall effect [5, 6]. This combination of predictive power and physical insight has profoundly shaped our understanding of quantum matter and continues to guide the discovery of new phases. Throughout this thesis, effective one-body theories serve as a common lens through which a range of interacting quantum systems of electrons is investigated.

Among the most successful approaches of this kind is Density Functional Theory (DFT) [7, 8], which has become a standard framework for the ab-initio description of solids. Through the Kohn–Sham construction, the interacting electron problem is mapped onto an auxiliary system of non-interacting particles moving in an effective potential, chosen to reproduce the exact ground state density. In practice, this framework enables quantitative predictions of structural, electronic, and magnetic properties across a broad range of materials, playing a central role in modern computational materials discovery. One output of this construction is a set of Bloch bands that provide an effective single-particle description of the solid, from which a wealth of observable properties can be straightforwardly computed. In recent years, this perspective has

proven particularly powerful in the study of topological phases, where geometric and topological quantities such as the Berry curvature [9, 10] and the Chern numbers [11] are determined by the wavefunctions of the occupied bands, connecting measurable responses to the global structure of the electronic band-structure [6, 12].

The success of these approaches raises a fundamental question: to what extent can a one-body picture survive in the presence of strong electron–electron interactions? Landau’s theory of Fermi liquids provides a partial answer. It shows that the low-energy excitations of a broad class of interacting metals can be described in terms of long-lived quasiparticles. Although their masses, lifetimes, and mutual interactions are strongly renormalized, these quasiparticles retain their fermionic character and provide an effective low-energy description in terms of weakly interacting quasiparticles.

However, when interaction energies become comparable to or larger than the electronic bandwidth, the quasiparticle picture can break down and qualitatively new phenomena emerge. Mott insulators are a paradigmatic example [13–15]: despite the presence of partially filled bands, strong local interactions suppress charge transport and produce an insulating state that cannot be understood within conventional band theory. Upon doping, coherent quasiparticles may partially re-emerge, and the resulting metallic phases can display pseudogaps, unconventional superconductivity, and signatures of fractionalization [16–19]. The interplay between strong correlations and non-trivial band topology further enlarges this landscape, giving rise to phases such as topological Mott insulators [20, 21] and fractionalized topological states [22–25].

A major advance in the theoretical description of strongly correlated electrons was the development of Dynamical Mean-Field Theory (DMFT) [26]. Rather than relying directly on renormalized quasiparticle bands, DMFT is formulated in terms of the interacting single-particle Green’s function. Its frequency dependence captures both coherent low-energy excitations and incoherent high-energy features, including the Hubbard bands characteristic of strongly correlated materials. Furthermore, while the poles of the Green’s function describe propagating electron-like quasiparticles, its full analytic structure contains even richer information about correlated states, such as the emergence of zeros, a hallmark of Mott insulators.

The single-particle spectral function, obtained from the imaginary part of the retarded Green’s function on the real-frequency axis, can be accessed experimentally through angle-resolved photoemission spectroscopy (ARPES). In a conventional metal, a narrow spectral peak near the chemical potential signals the presence of a coherent quasiparticle with finite overlap with the physical electron. Conversely, the suppression or disappearance of this peak is usually associated with the breakdown of the quasiparticle picture. This identification, however, has an intrinsic limitation: it probes only excitations that couple directly to the electron operator. In a fractionalized state, low-energy fermionic excitations may carry spin and entropy without carrying electric charge. Such excitations may form a Fermi surface and produce metal-like thermodynamic or heat-transport signatures, while leaving no quasiparticle pole in the physical electron Green’s function. The absence of an electron-like spectral peak therefore does not necessarily imply the absence of an underlying quasiparticle picture.

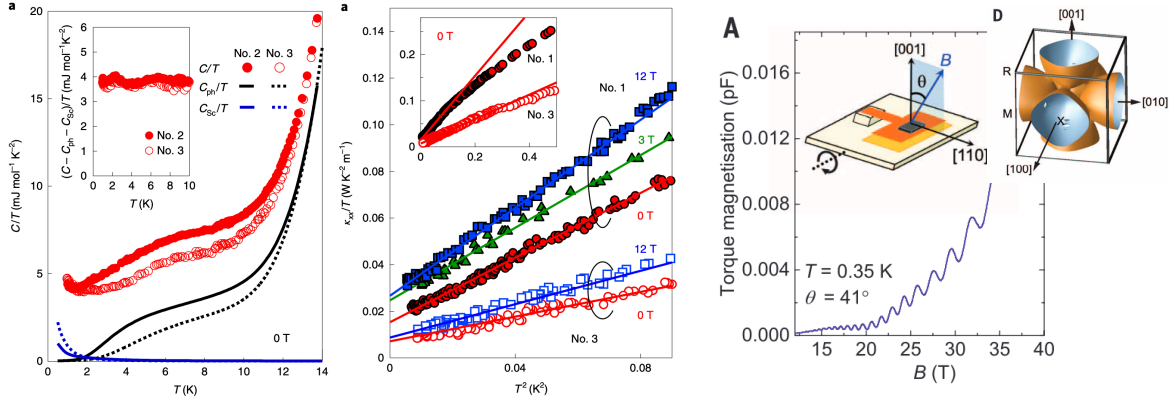


Figure 1: Signatures of charge-neutral fermionic excitations in electrically insulating Kondo insulators. **(a)** Heat capacity of YbB₁₂: once phonon and Schottky contributions are subtracted, the quasiparticle term C_{qp}/T (inset) stays finite as $T \rightarrow 0$, i.e. a specific heat linear in temperature, the hallmark of gapless fermionic excitations. **(b)** Thermal conductivity of YbB₁₂ vs T^2 at zero and finite field: the residual linear term κ_{xx}^0/T surviving as $T \rightarrow 0$ reveals itinerant heat carriers and a strong violation of the Wiedemann–Franz law – a charge insulator that is simultaneously a thermal metal. Panels (a,b) are adapted from Ref. [27]. **(c)** Quantum oscillations in the magnetic torque of SmB₆ against a quadratic background; the inset shows the three-dimensional Fermi surface reconstructed from the oscillation frequencies. Adapted from Ref. [28].

Some strongly correlated insulators display precisely this puzzling phenomenology. Despite the absence of quasiparticle peaks in ARPES and the presence of an electrical transport gap, they exhibit thermodynamic and magnetic responses characteristic of a Fermi liquid: a specific heat and thermal conductivity linear in temperature (Fig. 1a,b) [27], or a Pauli-like magnetic susceptibility [29]. In some cases, quantum oscillations have also been observed (Fig. 1c) [28], suggesting the presence of a well-defined Fermi surface of charge-neutral excitations despite the electrically insulating behavior. This dichotomy has been reported, for example, in the correlated Kondo insulators SmB₆ and YbB₁₂. Similarly, the layered Mott insulator 1T-TaS₂ displays a large low-temperature paramagnetic response without evidence of magnetic ordering or freezing. Measurements of its heat capacity and thermal conductivity have further motivated interpretations in terms of gapless spin excitations, possibly including itinerant spinons, although the experimental evidence for a spinon Fermi surface remains debated.

The challenge posed by these systems extends beyond the breakdown of conventional electron quasiparticles. Coherent, or quasiparticle-like, fermionic degrees of freedom may persist even when they are neither adiabatically connected to non-interacting electrons nor represented by poles of the physical electron Green’s function. Such excitations lie outside the scope of conventional band theory and may be revealed in the interacting electron Green’s function only indirectly, for instance through its zeros, corresponding to singularities of the self-energy. The central question is therefore whether

these systems admit an effective one-body description and, if so, which emergent degrees of freedom provide its appropriate basis.

This thesis investigates that question by developing and applying effective one-body frameworks for fermionic excitations beyond the conventional electron-quasiparticle paradigm. Instead of postulating adiabatic continuity with a non-interacting reference system, these frameworks derive the relevant quasiparticle structure from a non-perturbative treatment of the underlying many-body problem. The aim is to determine the conditions under which a one-body description remains valid in strongly correlated electron systems, to characterize the unconventional and potentially fractionalized fermionic excitations it supports, and to identify the observable signatures through which those excitations can be detected.

Exciton condensation driven by bound states of Green's function zeros

The first chapter of this thesis follows the interaction-driven evolution of a quantum spin Hall insulator into a Mott insulator. In the weakly correlated regime the relevant one-body structure is provided by the poles of the single-particle Green's function, continuously connected to the Bloch bands of the noninteracting system. Approaching the Mott transition, however, poles of the self-energy generate zeros of the Green's function, conventionally read as a mere suppression of electronic spectral weight. In Chapter 1, based on the work published in Ref. [30], we argue that the richer structure of the zeros can also provide an emergent low-energy quasiparticle picture, offering insight into the collective phenomena that arise in proximity to a Mott insulator.

We consider an interacting Bernevig–Hughes–Zhang model [31], in which two orbitals of opposite parity produce a quantum spin Hall phase through band inversion. Local Coulomb interactions are treated within the dynamical cluster approximation [32]. The inclusion of short-range spatial correlations allows the self-energy, and hence the Green's function zeros, to acquire a nontrivial momentum dependence. This makes it possible to follow both poles and zeros as dispersive objects across the transition and to study their relation to the competing symmetry-broken phases.

When all symmetries are enforced, dispersive bands of Green's function zeros appear already on the correlated quantum spin Hall side of the Mott transition. They co-exist with the valence and conduction bands formed by poles, producing a regime in which the interacting topology involves both structures. The corresponding boundary spectrum contains conventional electronic edge states together with chiral edge zeros. Upon entering the Mott phase, the physical electron spectrum separates into lower and upper Hubbard bands, while dispersive zero bands remain within the resulting charge gap. These zero bands can retain a nontrivial topology before becoming topologically trivial deeper in the Mott regime towards the atomic limit.

When symmetry breaking is allowed, a nontopological excitonic insulator intrudes be-

tween the quantum spin Hall and Mott phases [33, 34]. It is characterized by a spontaneous spin-triplet condensate between the opposite parity orbitals, thus breaking inversion, time-reversal and spin-rotation symmetry. Remarkably, the transitions between these insulators are continuous, thus requiring an excitonic mode that softens and condenses at the boundaries of the excitonic phase. On the quantum spin Hall side the soft mode is conventional: an electron in the conduction band and a hole in the valence band form a bound state due to the residual Coulomb interaction and condenses as the single-particle gap becomes small. Entering the excitonic phase, the single-particle gap increases, as expected from the level repulsion produced by exciton condensation (Fig. 1.11). On the Mott side, instead, the lower and upper Hubbard bands remain separated by a large charge gap, and an exciton between them would require a huge binding energy to soften at the transition. Furthermore, the single-particle gap decreases continuously across the transition, without any sign of a level repulsion.

To get a complementary perspective on the excitonic instability of the Mott phase, we turn to the finer analytic structure of the Green’s function, and in particular to its zeros. It is convenient to encode this information into an effective quasiparticle Hamiltonian, extracted from the low-frequency Green’s function, that treats poles and zeros on an equal footing. In the weakly correlated regime its bands coincide with the ordinary electronic bands, whereas in the Mott regime they track the dispersive bands of Green’s function zeros, and they evolve smoothly across the whole quantum spin Hall–excitonic–Mott sequence, providing a common description of the three phases. On the quantum spin Hall side the gap of these quasiparticle bands follows the single-particle one, so that the two agree. On the Mott side, instead, they part ways: the physical single-particle gap continuously decreases on entering the excitonic phase, showing no sign of level repulsion, whereas the quasiparticle gap recovers the level repulsion expected on entering the excitonic insulator, while remaining throughout much smaller than the Mott gap. Interpreted through the lens of this quasiparticle picture, it is tempting to argue that the mode that softens on the Mott side is not a bound state between the lower and upper Hubbard bands, but of effective quasiparticle and quasihole excitations associated with the bands of Green’s function zeros.

This chapter therefore provides a first example where the breakdown of the conventional band picture in a Mott insulator does not preclude an effective quasiparticle description. In the present case, the poles of the physical Green’s function still encode the Hubbard bands physics, but they no longer exhaust its low-energy properties: the zeros must be inspected as well. Although these zeros are not related to coherent electron-like quasiparticles, our results indicate that they retain quantum numbers such as parity, can carry topology, produce boundary signatures, and anticipate a collective instability. In this sense, Green’s function zeros may provide an effective description of hidden fermionic degrees of freedom in a Mott insulator, whose bound states can drive exciton condensation.

Fermi-liquid corrections to the intrinsic anomalous Hall conductivity of topological metals

The second chapter investigates how residual interactions among Landau quasiparticles affect the intrinsic anomalous Hall conductivity (AHC) of a topological metal. In a noninteracting crystal, the intrinsic AHC is conventionally expressed as an integral of the Berry curvature over the occupied Bloch states. Haldane showed, however, that in a metal its nonquantized part can be recast as a Fermi surface property, up to contributions associated with completely filled bands [35]. This observation places the intrinsic AHC within the domain of Fermi-liquid theory and raises a central question: is the Hall conductivity fully determined by the Berry curvature of the quasiparticle bands, or do the residual interactions among quasiparticles provide an additional contribution? The work presented in Chapter 2, based on Ref. [36], addresses this question.

We formulate the problem within a multiband extension of Landau Fermi-liquid theory, exploiting its correspondence with an interacting quasiparticle Hamiltonian treated within Hartree–Fock plus random phase approximation [37–39]. The Ward–Takahashi identities fix the current vertex in the q -limit, obtained by taking the transferred frequency $\omega \rightarrow 0$ before the transferred momentum $\mathbf{q} \rightarrow 0$, as $\hat{J}^q(\mathbf{k}) = \nabla_{\mathbf{k}} \hat{H}_*(\mathbf{k})$, with $\hat{H}_*$ the quasiparticle Hamiltonian. Substituting this vertex into the Kubo formula for the Hall conductivity reproduces the familiar TKNN expression [6], now written in terms of the Berry curvature of the quasiparticle bands. Within the present framework, this result is exact for a fully gapped system, where the q -limit and the ω -limit, obtained by taking $\mathbf{q} \rightarrow 0$ before $\omega \rightarrow 0$, commute. However, in presence of a Fermi or Luttinger surface the two limits no longer commute due to the nonanalyticity of the response functions at $(\omega, \mathbf{q}) = 0$. The dynamic current vertex $\hat{J}^\omega(\mathbf{k})$, required in the Kubo formula, differs from $\hat{J}^q(\mathbf{k})$ and acquires vertex corrections generated by the residual interaction among Landau quasiparticles on the Fermi surface.

Using the dressed current vertex in the ω -limit, we derive a general expression for the intrinsic anomalous Hall conductivity. The Berry curvature is now constructed from the dynamic current vertex rather than solely from the quasiparticle eigenstates. Consequently, the Hall conductivity contains not only the geometric contribution associated with the quasiparticle bands, but also genuine Fermi-liquid corrections originating from residual quasiparticle interactions. Although these corrections arise entirely from quasiparticles at the Fermi surface, they renormalize the full intrinsic Hall response.

We illustrate this result in a spin-polarized and doped Bernevig–Hughes–Zhang model, describing a two-dimensional topological metal with broken time-reversal symmetry. For a representative class of Landau interactions, the anomalous Hall conductivity takes the simple form

$$\sigma^H = \sigma_0^H \left(1 + \frac{F_2^1}{2} \right),$$

where σ_0^H is the Berry curvature contribution of the quasiparticle bands and F_2^1 is an appropriate Fermi-surface average of the Landau f -parameters. This renormalization

factor is the Hall counterpart of the familiar Fermi-liquid correction to the current and Drude weight in longitudinal transport.

The main message of this chapter is that the effective quasiparticle Hamiltonian does not, by itself, exhaust the transport predictions of Fermi-liquid theory. In a topological metal, the residual interactions among quasiparticles on the Fermi surface renormalize the current vertex and thereby modify the intrinsic anomalous Hall conductivity. Once the corresponding vertex corrections are included, Landau theory naturally accounts for deviations from the Hall response obtained by integrating the Berry curvature of the quasiparticle bands alone. The effective quasiparticle description therefore remains the appropriate starting point for characterizing the low-energy electronic structure of topological metals, but it must be supplemented by the residual interactions, encoded in the Landau f -parameters, when computing transport properties.

Static and dynamical properties of a strong-coupling impurity solver for dynamical mean field theory

The effective one-body descriptions developed in this thesis rely on extracting the relevant many-body information from simplified models that retain the essential physics of the systems under investigation. Dynamical mean-field theory (DMFT) is among the most successful non-perturbative frameworks for this purpose. It maps a correlated lattice model onto a quantum impurity coupled to a self-consistently determined bath and it is exact in the limit of infinite lattice coordination [26, 40]. The resulting impurity problem remains fully interacting, and its solution is the central computational step of any DMFT calculation. The choice of impurity solver therefore determines both the accuracy of the results and the range of observables that can be reliably computed. Building on Ref. [41], in Chapter 3 we present and discuss a deterministic strong-coupling impurity solver that complements, and in some regimes outperforms, the stochastic Monte Carlo methods that currently dominate the field.

The method leverages a pseudoparticle representation of the local impurity many-body states. This formulation yields a controlled bold expansion in the impurity–bath hybridization, with the atomic limit as the unperturbed reference point [42, 43]. Crucially, the partition function is evaluated explicitly rather than estimated through stochastic sampling. Static, dynamical, and thermodynamic observables can therefore be obtained within the same calculation. In particular, the method provides direct access to the impurity and lattice free energies. This is a major advantage over stochastic solvers, for which free energies usually require costly thermodynamic integration and a large number of independent self-consistent calculations. Directly computing the free energy makes it possible to compare the thermodynamic stability of competing DMFT solutions and to determine the phase transition itself, rather than only the boundaries of the coexistence region.

We benchmark the solver on the single-band Hubbard model on the Bethe lattice, across

the metal-to-Mott-insulator transition and down to low temperatures. Convergence with the expansion order is fast in the Mott insulating phase, adiabatically connected to the atomic limit, where low-order expansions already agree with continuous-time quantum Monte Carlo results within their statistical accuracy, while requiring orders of magnitude less computational effort. In the metallic phase convergence is slower and non-monotonic, as the low-order truncation inherits the over-screened, non-Fermi-liquid low-energy behavior of the non-crossing approximation. Nevertheless, static and thermodynamic observables converge substantially faster than dynamical quantities. The solver accurately reproduces the double occupancy, energy per site, and entropy. It captures both the residual entropy $S = \ln 2$ of the paramagnetic Mott insulator within DMFT and the Pomeranchuk effect in the correlated metal. Most importantly, the explicit free-energy balance identifies which of the coexisting metallic and insulating solutions is thermodynamically stable. It thus locates the first-order transition line directly, without relying on an indirect reconstruction of the thermodynamic potential. The same framework applies naturally away from half-filling.

The solver presented in Chapter 3 holds promising potential in regimes where stochastic methods become prohibitively expensive. This occurs, for example, in multiorbital and spin-orbit coupled models, where the sign problem severely restricts the accessible temperature range. By extending controlled calculations into these regimes, more efficient impurity solvers broaden the range of correlated systems that can be investigated. Their underlying physical mechanisms can then be analyzed through the effective one-body descriptions that form the common thread of this thesis.

Topology, correlations and magnetism with the ghost-Gutzwiller Ansatz

The fourth chapter explores how strong electronic correlations modify the topological properties of quantum materials, often giving rise to intriguing phenomena with no analogue in the noninteracting limit. Addressing this problem requires bridging the language gap between topological band theory, naturally formulated in terms of single-particle Bloch states, and the many-body language of strongly correlated systems, which usually eludes a one-body description. Based on Ref. [44], Chapter 4 asks whether the ghost-Gutzwiller (gGut) ansatz can bridge this gap. This framework restores an effective band-structure description that incorporates nonperturbative correlation effects while retaining a transparent one-body interpretation convenient for a topological analysis.

The variational gGut wave function is built starting from an uncorrelated Fock state, which is the ground state of an auxiliary quasiparticle Hamiltonian, $H_{\text{qp}}(\mathbf{k})$. In addition to the physical electronic orbitals, the quasiparticle Hilbert space contains auxiliary "ghost" orbitals: They provide the variational flexibility required to reproduce the frequency dependence of the electronic self-energy and the transfer of spectral weight

from coherent quasiparticle bands to high-energy Hubbard bands. Within the gGut approximation, the physical electron Green’s function is obtained by projecting the resolvent of this enlarged quasiparticle Hamiltonian onto the physical electronic sector. The auxiliary band structure therefore constitutes an effective one-body representation of the interacting problem.

We establish the topological meaning of this auxiliary description starting from the spectral representation of the physical Green’s function within the gGut formalism. We show that the topological invariant of an interacting insulating state can be obtained from the quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$. More precisely, the sum of Chern numbers of its occupied bands reproduces the invariant defined from the winding number of the interacting Green’s function [45–47]. The quasiparticle Hamiltonian is therefore not merely a convenient parametrization of the variational state: its eigenvectors retain the topological information of the interacting system and make it possible to apply the geometrical tools of band theory, including Berry curvatures, Chern numbers, and bulk–boundary relations, to a nonperturbative variational description of strongly correlated topological phases.

We test this construction in the interacting Bernevig–Hughes–Zhang model, where we follow the correlation-driven evolution of a quantum spin Hall insulator towards a Mott insulator. The enlarged quasiparticle Hamiltonian captures the redistribution of spectral weight across the transition while retaining an effective band interpretation of both the low-energy and high-energy features of the spectrum: In the weakly correlated regime, the relevant topological bands are continuously connected to the physical electronic bands; As the interaction is increased, additional auxiliary bands acquire physical spectral weight and develop into the lower and upper Hubbard bands.

The most striking result of this work concerns the topology of the high-energy Hubbard bands. Rather than being featureless incoherent excitations, we find that they may themselves acquire a nontrivial topology and support protected edge states despite lying far from the Fermi level. This establishes the existence of topological Hubbard bands, whose topological character is generally independent of that of the low-energy quasiparticle bands. Furthermore, leveraging the magnetic susceptibility of the paramagnetic Mott state, we show that a finite magnetization acts as an effective tuning parameter for the topological character of these high-energy Hubbard bands.

We can thus conclude that the gGut framework provides a simple and physically transparent route to capture the interplay of strong correlations, topology, and magnetism in quantum materials. It retains an effective band description even in nonperturbative regimes, accounting for the emergence of topological Hubbard bands and their tunability with magnetic fields. More broadly, the gGut construction provides a bridge between the language of band topology and the many-body physics of correlated electrons.

Fractionalized Fermi liquids with the ghost-Gutzwiller Ansatz

The fifth and last chapter takes the ghost-Gutzwiller construction introduced in Chapter 4 one step further. Here, we investigate whether the same framework can account for dispersive fermionic excitations having vanishing overlap with the physical electron. This scenario is theoretically realized in fractionalized Fermi liquids, conventionally denoted by FL^* , in which conventional electron-like quasiparticles coexist with neutral spin-1/2 excitations. In the work presented in Chapter 5, based on Ref. [48], we show that a FL^* phase emerges in the single-band t - J model through a simple ghost-Gutzwiller Ansatz, optimized at the cost of a mean-field calculation.

Applying the gGut method to the t - J model first requires extending the formalism to treat the non-local spin-exchange interaction. To this end, we introduce a spin-renormalization matrix that maps the physical exchange term onto the auxiliary quasiparticles, in analogy with the renormalization of the electronic hopping. The non-local character of the exchange interaction is essential: it allows the neutral quasiparticles to acquire a genuine dispersion and generates a momentum-dependent electronic self-energy.

Then, within a minimal construction involving only two auxiliary orbitals, we show that this variational ansatz admits two physically relevant limits. The first simply reproduces the conventional Gutzwiller approximation. In its normal state, it describes an ordinary Fermi liquid in which the doped charge is carried by quasiparticles with finite physical electron spectral weight. Upon lowering the temperature, this Fermi liquid becomes unstable toward d -wave superconductivity and develops a finite order parameter Δ_{SC} . The second possibility realizes a FL^* phase, in which one auxiliary quasiparticle band remains half-filled, but has vanishing physical electron spectral weight. Through the spin-renormalization matrix, these quasiparticles nevertheless carry spin and can therefore be identified as neutral dispersive spinons. The second quasiparticle band, by contrast, carries both spin and electric charge and forms a small hole-like Fermi surface whose volume violates Luttinger's theorem.

To investigate the competition between the different phases listed above, we further extend the variational framework to finite temperature. Since the entropy of a Gutzwiller projected density matrix is not directly accessible, we derive a computable lower bound that becomes exact both at zero temperature and in the infinite-temperature limit. The resulting temperature-doping phase diagram displays the key qualitative features of cuprates: a low-doping FL^* regime, a d -wave superconducting dome, and an overdoped conventional Fermi liquid. Within the fractionalized regime, the spinons form a π -flux state below a characteristic temperature T^* , which may be associated with the onset of pseudogap behavior. Although this state is gauge equivalent to a d -wave state at half-filling, it does not by itself imply physical superconductivity, since the paired quasiparticles carry no physical electron spectral weight. A physical superconducting order parameter appears only when the paired excitations recombine with the charged degrees of freedom and acquire a finite overlap with the physical electrons.

The main conclusion of this work is that the ghost-Gutzwiller Ansatz provides a simple variational description of a fractionalized Fermi liquid directly within a single-band t - J model of a doped Mott insulator. It captures the coexistence of conventional quasiparticles with hidden ones that are electrically neutral yet carry spin. More broadly, these results show that the auxiliary quasiparticles of the ghost-Gutzwiller construction need not merely reproduce the single-particle spectrum: they can also describe fractionalized excitations with no physical electron spectral weight. This opens the route to studying unconventional metals and correlated insulators with gapless neutral excitations within an effective quasiparticle picture.

CHAPTER 1

Exciton condensation driven by bound states of Green's function zeros

In this chapter, we investigate the interaction-driven evolution of a quantum spin Hall insulator within the dynamical cluster approximation. We discover that an excitonic insulator lies between the quantum spin Hall insulator at weak coupling and the Mott insulator at strong coupling. The single-particle spectrum clearly shows the transition from the quantum spin Hall insulator to the excitonic insulator, but it lacks evidence of the transition from the Mott insulator to the excitonic one. In this case, the evolution of the in-gap dispersive bands of Green's function zeros serves as a signature of the transition. As the Mott phase approaches the transition, the gap between these bands narrows, while entering the excitonic phase, the gap then grows. This behavior suggests that the excitons, which become soft at the transition, may actually represent bound states of valence and conduction bands of Green's function zeros. This chapter is based on Ref. [30].

Introduction

Upon increasing the electron-electron interaction strength, models of topological band insulators (TBIs) can be driven into supposedly trivial, non-symmetry-breaking correlated insulators (CIs) without the expected closing at the transition of the single-particle gap. Several ways have been found that allow circumventing the occurrence of a metal point between TBI and CI. The simplest and most direct is a discontinuous character of the transition [34, 49], but there seem to exist other more subtle routes connecting a TBI to a CI without crossing a metal.

For instance, a new insulating phase can intrude between TBI and CI that spontaneously breaks the symmetry which protects the topology. In the Bernevig-Hughes-Zhang (BHZ) model of quantum spin Hall insulators (QSHIs) [31], this phase describes a magnetoelectric excitonic insulator, which thus breaks parity and time reversal [33, 34]. As a matter of fact, exciton condensation is a logical outcome when the single-particle gap gets small around the TBI-CI transition. Indeed, there is evidence of indirect-exciton condensation in monolayer WTe₂ [50], which leads to a topological

insulator that breaks time-reversal symmetry.

A further and rather exotic scenario is that the TBI-to-CI transition is direct and continuous, the single-particle gap remains finite and smooth, and, yet, a gapless point emerges within the particle-hole and/or particle-particle spectra. Slagle, You, and Xu [51] have studied an AA-stacked honeycomb-lattice bilayer, where each layer is described by a Kane-Mele model [52] of a QSHI plus an onsite Hubbard U . In turn the two layers are coupled to each other through an antiferromagnetic exchange J . Upon increasing U , at large $J/U = 2$, they find a continuous transition from the QSHI to a trivial CI that is simply a collection of interlayer singlets. At the transition, the single-particle gap remains finite, whereas the spin gap as well as the gap to adding or removing two electrons in the inter-layer spin-singlet channel vanish. This result raises an interesting issue. Indeed, the QSHI phase is characterized by a topological invariant $C_{\uparrow} = -C_{\downarrow} = \pm 1$, with C_{σ} the Chern number of the spin- σ band, which is also the winding number $W(G_{\uparrow}) = -W(G_{\downarrow})$ of the map $(\epsilon, \mathbf{k}) \mapsto G_{\uparrow}(i\epsilon, \mathbf{k}) \in GL(2, \mathbb{C})$ [45, 53]. Here $G_{\uparrow}(i\epsilon, \mathbf{k})$ is the spin-up Green's function in Matsubara frequencies ϵ , and $\mathbf{k}$ the two-dimensional momentum. Remarkably, the winding number retains the same quantized value on both sides of the transition [51], which in turn implies that the topological bands of poles of the QSHI Green's function transform into topological bands of zeros in the CI [47, 54–57]. However, while the topological invariant $W(G_{\uparrow}) - W(G_{\downarrow})$ corresponds to the quantized spin Hall conductance $C_{\uparrow} - C_{\downarrow}$ in the QSHI, this correspondence fails in the CI, which is a trivial collection of inter-layer singlets and consequently has vanishing spin Hall conductance. In other words, the winding number, though it is a topological invariant, is not necessarily equivalent to the quantized Hall or spin-Hall conductance [36, 47, 58].

How the transmutation of topological poles into topological zeros occurs across the transition is known only in rather artificial cases [56]. It is also unclear whether such a change of analyticity bears any signature of the vanishing spin and charge- $2e$ gaps, even though it is tempting to argue that their closing, despite the finite charge- e gap, corresponds to a Dirac-type touching of the bands of zeros — and thus to the emergence of a Luttinger surface [59], reduced to just two points in that specific case.

The zeros of the Green's function, whose locus in momentum space defines a Luttinger surface, have no counterpart in a non-interacting band picture and are a distinctive fingerprint of Mott insulators (MIs) where they accompany the opening of a charge gap with no symmetry breaking. Whether they are genuine physical objects or mere mathematical artifacts has been the subject of an intense debate. A growing body of work suggests that they should be taken seriously: zeros can carry their own topological invariants, sustain edge states, and be understood as the fingerprint of *hidden* quasiparticles, i.e. coherent low-energy excitations that are invisible in the single-particle spectrum because of a vanishing spectral weight, yet still able to transport spin and entropy and to shape the response functions [57, 59–61].

In this chapter both routes come into play, and their interplay raises a particularly intriguing question. Single-site dynamical mean-field theory [26] already shows that an excitonic insulator intrudes between the quantum spin Hall insulator and the MI, and

that the transition between the excitonic and the Mott insulators is continuous [34]. A continuous transition requires an excitonic mode that softens inside the MI and condenses at the transition. However, the single-particle gap remains large and smooth across it. Therefore, the exciton softening appears unrelated to the Mott gap separating the lower and upper Hubbard bands. Since that gap harbors in-gap bands of Green's function zeros, it is tempting to conjecture that these excitons could be better regarded as bound states between the valence and conduction bands of zeros, rather than between the Hubbard bands. To investigate this scenario, we study the BHZ model by means of the dynamical cluster approximation [32], which retains the non-local correlations required to give the bands of zeros a genuine dispersion. We find that bands of zeros emerge already on the QSHI side of the transition, where they give rise to a topological pseudogap insulator hosting both chiral edge poles and chiral edge zeros, and that they survive across the continuous Mott transition. Most importantly, by tracking the quasiparticle Hamiltonian that treats poles and zeros on the same footing, we provide evidence that the soft exciton indeed looks like a bound state of Green's function zeros.

1.1 A simple model for correlated quantum spin Hall insulators

A minimal lattice model realization of a two-dimensional topological insulator was introduced by Bernevig, Hughes and Zhang (BHZ) to describe the quantum spin Hall phase of HgTe quantum wells [31]. The BHZ model captures the essential ingredients of band topology, and serves as the natural starting point to investigate how electron-electron interactions can drive a quantum spin Hall insulator (QSHI) into a correlated insulating phase. In this section we introduce the model in its non-interacting form, discuss its symmetries and topological properties, and then consider a local Coulomb-like interaction compatible with the symmetries of the model. The leading particle-hole instabilities can be identified already at the level of the bare scattering amplitudes, and anticipate the excitonic phases that we will study in detail in the rest of the chapter.

1.1.1 The non-interacting BHZ Hamiltonian

The BHZ model involves two spinful Wannier orbitals per unit cell. The first transforms like an s orbital, $|\ell = 0, \sigma\rangle \equiv |s \sigma\rangle$, with $\sigma = \uparrow, \downarrow$ the spin projection along z , while the second is built from the $J = 3/2$, $J_z = \pm 3/2$ spin-orbit coupled combinations of p orbitals,

$$|p_x + ip_y, \uparrow\rangle \equiv |p \uparrow\rangle, \quad |p_x - ip_y, \downarrow\rangle \equiv |p \downarrow\rangle. \quad (1.1)$$

We introduce two sets of Pauli matrices, σ_a and τ_a with $a = 0, \dots, 3$ and $a = 0$ denoting the identity, acting respectively on the spin and orbital degrees of freedom. In terms

of the four-component spinor

$$\Psi_{\mathbf{k}}^\dagger = \left(s_{\mathbf{k}\uparrow}^\dagger, s_{\mathbf{k}\downarrow}^\dagger, p_{\mathbf{k}\uparrow}^\dagger, p_{\mathbf{k}\downarrow}^\dagger \right), \quad (1.2)$$

the non-interacting Hamiltonian on a square lattice, including on-site and nearest-neighbour terms [62], reads

$$H_0 = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \hat{H}_0(\mathbf{k}) \Psi_{\mathbf{k}}, \quad (1.3)$$

with the 4×4 Bloch matrix

$$\hat{H}_0(\mathbf{k}) = \left(M - t(\cos k_x + \cos k_y) \right) \sigma_0 \otimes \tau_3 + \lambda \sin k_x \sigma_3 \otimes \tau_1 - \lambda \sin k_y \sigma_0 \otimes \tau_2. \quad (1.4)$$

Hereafter we set $t = 1$ as the unit of energy, $\lambda = 0.3$, and work at half filling, i.e. two electrons per site. Without loss of generality we take $M \geq 0$.

The spectrum of $\hat{H}_0(\mathbf{k})$ consists of two doubly degenerate bands, separated by a direct gap that closes at two distinct values of the mass parameter: at $M = 2$, where the gap closes at $\Gamma = (0, 0)$ with a single Dirac cone, and at $M = 0$, where the gap closes simultaneously at the two inequivalent points $X = (\pi, 0)$ and $Y = (0, \pi)$. For $0 < M < 2$ the model describes a QSHI, while for $M > 2$ it describes a trivial band insulator. At the high-symmetry points $\Gamma = (0, 0)$, $M = (\pi, \pi)$, $X = (\pi, 0)$ and $Y = (0, \pi)$ the eigenstates have a well-defined orbital character, hence a well-defined parity under inversion: in the QSHI regime the valence and conduction bands exchange their dominant s or p character moving from Γ to the Brillouin zone boundary, while in the trivial regime each band keeps a single orbital character throughout the Brillouin zone, as illustrated in Fig. 1.1.

The Hamiltonian (1.4) is invariant under inversion $\mathcal{I}$, time-reversal $\mathcal{T}$, and spatial $\mathcal{C}_4$ rotation symmetries, represented by

$$\mathcal{I}: \hat{H}_0(\mathbf{k}) = \sigma_0 \otimes \tau_3 \hat{H}_0(-\mathbf{k}) \sigma_0 \otimes \tau_3, \quad (1.5)$$

$$\mathcal{T}: \hat{H}_0(\mathbf{k}) = (-i\sigma_2 \otimes \tau_0) \hat{H}_0^*(-\mathbf{k}) (i\sigma_2 \otimes \tau_0), \quad (1.6)$$

$$\mathcal{C}_4: \hat{H}_0(\mathbf{k}) = e^{-i\frac{\pi}{2}L_3} \hat{H}_0(\mathcal{C}_4(\mathbf{k})) e^{i\frac{\pi}{2}L_3}, \quad (1.7)$$

where $\mathcal{C}_4(\mathbf{k}) = (-k_y, k_x)$, and the z -component of the angular momentum operator is

$$L_3 = \sigma_3 \otimes \frac{\tau_0 - \tau_3}{2}. \quad (1.8)$$

The periodic model (1.4) is furthermore symmetric under spin $U(1)$ rotations around the z -axis that plays an important role in protecting the topology. Indeed, it allows the definition of a robust $\mathbb{Z}_2$ invariant ν as the difference of the Chern numbers of the two spin sectors [52]:

$$\nu = \frac{C_\uparrow - C_\downarrow}{2} \mod 2. \quad (1.9)$$

We mention that spin $U(1)$ symmetry is actually a consequence of $\mathcal{C}_4$ symmetry, which is only approximate in zinc-blende HgTe. The fact that this symmetry is not exact will

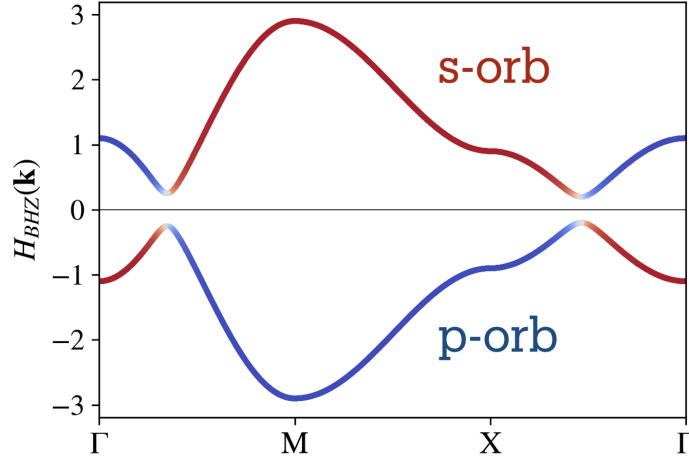


Figure 1.1: Band structure of the non-interacting BHZ Hamiltonian (1.4) along the high-symmetry path $\Gamma \rightarrow M \rightarrow X \rightarrow \Gamma$ of the square lattice Brillouin zone, for $\lambda = 0.3$ and a representative value of the mass parameter M corresponding to a QSHI phase. Each band is doubly degenerate. The colour encodes the dominant orbital character (s or p) of the eigenstates: in the QSHI regime the valence and conduction bands exchange their dominant character between Γ and the Brillouin zone boundary.

be relevant for the excitonic insulator discussed below, whose order parameter breaks precisely the spin $U(1)$. As we shall see in Sec. 1.5.1, this is what allows a genuine finite-temperature exciton-condensation transition to take place.

With our choice of parameters, the QSHI phase $0 < M < 2$ is characterized by spin-resolved Chern numbers $C_{\uparrow} - C_{\downarrow} = 2$, which can also be expressed as the winding number of the Green's function in Matsubara frequencies [63], a viewpoint introduced in Sec. 1.3.2 that will become central in the analysis of the strongly correlated regime.

1.1.2 Local interaction and atomic Mott limits

To investigate the effects of correlations, we consider an interaction Hamiltonian obtained by projecting the local Coulomb repulsion onto the s and p Wannier orbitals, retaining all the terms compatible with the symmetries of the orbitals [33]. We thus consider

$$H_{\text{int}} = \sum_{\mathbf{R}} H_{\text{int}}(\mathbf{R}), \quad (1.10)$$

with

$$H_{\text{int}}(\mathbf{R}) = U_s n_{s\mathbf{R}\uparrow} n_{s\mathbf{R}\downarrow} + U_p n_{p\mathbf{R}\uparrow} n_{p\mathbf{R}\downarrow} + V n_{s\mathbf{R}} n_{p\mathbf{R}} + H_{\text{dip}}(\mathbf{R}), \quad (1.11)$$

where $n_{a\mathbf{R}\sigma} = a_{\mathbf{R}\sigma}^\dagger a_{\mathbf{R}\sigma}$ for $a = s, p$, $n_{a\mathbf{R}} = n_{a\mathbf{R}\uparrow} + n_{a\mathbf{R}\downarrow}$, and $H_{\text{dip}}(\mathbf{R})$ is the dipole-dipole component of the multipole expansion of the Coulomb interaction, which is allowed by

symmetry on this orbital basis. Explicitly,

$$\begin{aligned}
 H_{\text{dip}}(\mathbf{R}) &= \frac{J}{2} \left[(\Psi_{\mathbf{R}}^\dagger \sigma_0 \otimes \tau_1 \Psi_{\mathbf{R}})^2 + (\Psi_{\mathbf{R}}^\dagger \sigma_3 \otimes \tau_2 \Psi_{\mathbf{R}})^2 \right] \\
 &= J \left(s_{\mathbf{R}\uparrow}^\dagger s_{\mathbf{R}\downarrow}^\dagger p_{\mathbf{R}\downarrow} p_{\mathbf{R}\uparrow} + p_{\mathbf{R}\uparrow}^\dagger p_{\mathbf{R}\downarrow}^\dagger s_{\mathbf{R}\downarrow} s_{\mathbf{R}\uparrow} \right. \\
 &\quad \left. + s_{\mathbf{R}\uparrow}^\dagger p_{\mathbf{R}\uparrow}^\dagger s_{\mathbf{R}\uparrow} p_{\mathbf{R}\uparrow} + s_{\mathbf{R}\downarrow}^\dagger p_{\mathbf{R}\downarrow}^\dagger s_{\mathbf{R}\downarrow} p_{\mathbf{R}\downarrow} \right). \tag{1.12}
 \end{aligned}$$

All couplings U_s , U_p , V and J are positive. To reduce the number of independent parameters, we set $U_s = U_p \equiv U$ in what follows. Under the assumption $\min(U_s, U_p) > V$, the interaction (1.11) enforces Hund's rules, so that the lowest-energy two-electron local configuration is a spin triplet with $S = 1$ and $S_z = \pm 1$. In the strong-coupling limit, this leads to a high-spin (hs) Mott insulator in which each site hosts one electron per orbital, locked into a magnetic triplet [64].

The hs-MI is expected to be unstable towards magnetic ordering of the local moments, which would prevent a direct transition into a paramagnetic Mott insulator that we aim to study. This motivates us to consider also a complementary setting in which a truly paramagnetic Mott phase can be stabilized, so as to test the robustness of our main conclusions against the specific nature of the Mott state. To this end, we also study the case $J < 0$, which is not allowed by the bare Coulomb interaction but can be generated dynamically when the electrons are strongly coupled to an infrared optical phonon mode, twofold degenerate by $\mathcal{C}_4$, and with normal coordinates $q_{1\mathbf{R}}$ and $q_{2\mathbf{R}}$,

$$H_{\text{el-ph}}(\mathbf{R}) = q_{1\mathbf{R}} (\Psi_{\mathbf{R}}^\dagger \sigma_0 \otimes \tau_1 \Psi_{\mathbf{R}}) + q_{2\mathbf{R}} (\Psi_{\mathbf{R}}^\dagger \sigma_3 \otimes \tau_2 \Psi_{\mathbf{R}}). \tag{1.13}$$

Integrating out the phonons and neglecting retardation effects, this generates an effective interaction of the same form as (1.12) but with a negative coupling $J' < 0$. When the phonon-mediated contribution overcomes the bare Hund's exchange, the two add up to an effective dipole-dipole term with $J \equiv J_{\text{Hund}} + J' < 0$. In this regime, the two-electron local ground state is twofold degenerate, comprising the configurations in which the two orbitals are singly occupied and coupled either in a spin singlet $S = 0$ or in the $S_z = 0$ component of the spin triplet. To make contact with the related bilayer model of Slagle, You and Xu [51], we lift this degeneracy by adding the term

$$\delta H_{\text{dip}}(\mathbf{R}) = -\delta J (s_{\mathbf{R}\uparrow}^\dagger p_{\mathbf{R}\downarrow}^\dagger s_{\mathbf{R}\downarrow} p_{\mathbf{R}\uparrow} + \text{h.c.}), \quad \delta J > 0, \tag{1.14}$$

which selects the interorbital singlet and thus stabilizes a non-magnetic, Van Vleck paramagnetic low-spin Mott insulator (ls-MI). We note that (1.14) explicitly breaks $\mathcal{C}_4$, since it is not invariant under the transformation $p_{\mathbf{R}\uparrow} \rightarrow i p_{\mathbf{R}\uparrow}$, $p_{\mathbf{R}\downarrow} \rightarrow -i p_{\mathbf{R}\downarrow}$.

A noticeable feature of the model at $J < 0$ and $\delta J > 0$ is that the ls-MI cannot physically support a finite spin Hall conductance, just like the model analyzed in [51]. Therefore, this model allows us to clearly distinguish the winding number from the observable spin Hall conductance. Furthermore, since the case with $J < 0$ behaves similarly to that with $J > 0$, we argue that also the hypothetical paramagnetic hs-MI has vanishing spin Hall conductance despite a quantized winding number. This

conclusion, which we can draw without explicitly calculating the spin Hall conductance, which is unfeasible within the dynamical cluster approximation, clarifies an open issue regarding the topological properties of the hs-MI [65].

1.1.3 Leading symmetry-breaking channels

A lot of insights on the interacting BHZ model can be gained looking at the set of accessible particle-hole instabilities. These can be classified by computing the bare scattering amplitudes $\Gamma_{\alpha\alpha}^0$ associated with the local bilinears $\Psi_{\mathbf{R}}^\dagger \sigma_\alpha \otimes \tau_a \Psi_{\mathbf{R}}$, and selecting those that are most negative [33, 34]. For $J > 0$, the leading symmetry-breaking channels are:

- (i) $\Gamma_{30}^0 = -(U + 2J)/4$, which tends to stabilize ferromagnetic or antiferromagnetic order with local magnetization parallel or antiparallel to z ;
- (ii) $\Gamma_{11}^0 = \Gamma_{21}^0 = -(V + 2J)/4$, degenerate because of the spin $U(1)$ symmetry, which drives an excitonic instability with order parameter

$$\Delta(\phi) = \cos \phi \langle \Psi_{\mathbf{R}}^\dagger \sigma_1 \otimes \tau_1 \Psi_{\mathbf{R}} \rangle + \sin \phi \langle \Psi_{\mathbf{R}}^\dagger \sigma_2 \otimes \tau_1 \Psi_{\mathbf{R}} \rangle. \quad (1.15)$$

The condensation of (1.15) breaks inversion, time-reversal, and spin $U(1)$ symmetries, and it gives rise to a magnetoelectric excitonic insulator [33, 34].

Since $U > V$, in the deep Mott regime the magnetic instability (i) is expected to prevail. However, as we shall see in the following sections, the excitonic instability (ii) is the one responsible for the emergence of an excitonic insulator (EI) intruding between the QSHI and the Mott insulator.

For $J < 0$, the dominant scattering amplitudes change accordingly:

- (i) $\Gamma_{33}^0 = -(U + 2|J|)/4$, which in the Mott regime favors an ordering of the local configurations $s_{\mathbf{R}\uparrow}^\dagger p_{\mathbf{R}\downarrow}^\dagger |0\rangle$ and $p_{\mathbf{R}\uparrow}^\dagger s_{\mathbf{R}\downarrow}^\dagger |0\rangle$;
- (ii) $\Gamma_{01}^0 = \Gamma_{32}^0 = -(V + 4|J|)/4$, degenerate by $\mathcal{C}_4$, which drives an excitonic instability.

Adding the term (1.14) stabilizes the interorbital spin singlet $\frac{1}{\sqrt{2}}(s_{\mathbf{R}\uparrow}^\dagger p_{\mathbf{R}\downarrow}^\dagger + p_{\mathbf{R}\uparrow}^\dagger s_{\mathbf{R}\downarrow}^\dagger) |0\rangle$ in the Mott phase, and the leading excitonic order parameter becomes

$$\Delta = \langle \Psi_{\mathbf{R}}^\dagger \sigma_0 \otimes \tau_1 \Psi_{\mathbf{R}} \rangle, \quad (1.16)$$

which breaks inversion but preserves time-reversal.

1.2 Exciton bound states softening into an excitonic insulator

The bare-scattering analysis of Sec. 1.1.3 singled out the exciton channel as a leading particle-hole instability of the interacting BHZ model. Whether this instability actually

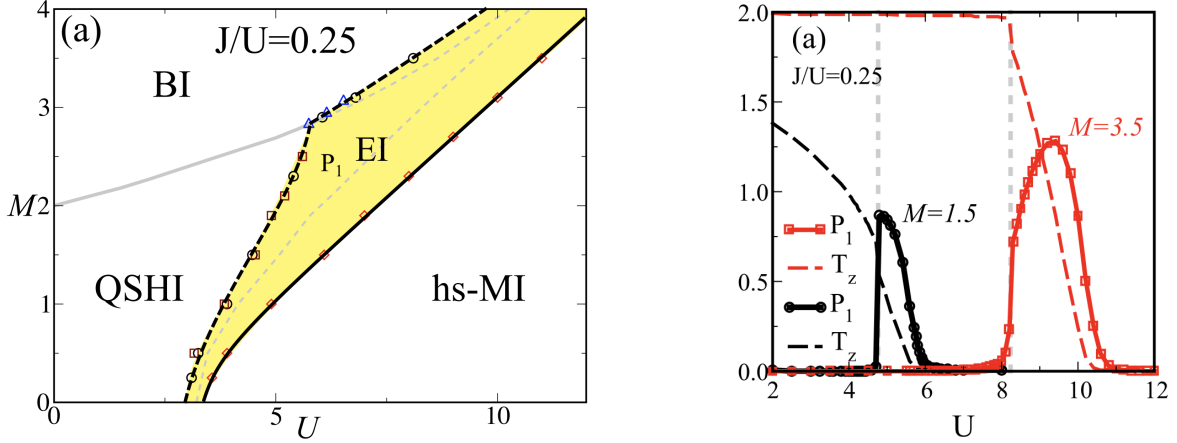


Figure 1.2: DMFT results for the interacting BHZ model at $J/U = 0.25$, adapted from Ref. [34]. Left panel: Phase diagram in the (U, M) plane. The excitonic insulator (yellow) intrudes between the QSHI and the high-spin Mott insulator. Dashed lines denote first-order, solid lines continuous transitions; in particular, the EI–MI boundary is continuous. Right panel: Excitonic order parameter $P_1 = \langle \Psi_{\mathbf{R}}^\dagger \sigma_1 \otimes \tau_1 \Psi_{\mathbf{R}} \rangle$ as a function of U at fixed M : the bell-shaped profile demonstrates the continuous character of the EI–MI transition (right edge), with P_1 closing smoothly as U grows into the Mott regime.

condenses into an ordered phase with a non-zero expectation value of (1.15) has been the subject of previous studies: At weak coupling, a Hartree-Fock plus Bethe-Salpeter equation analysis [33] showed that the order parameter (1.15) indeed condenses, giving rise to an EI that intrudes between the QSHI and the trivial band insulator. Because the condensate breaks the time-reversal symmetry protecting the topology of the original periodic model (1.4), the EI provides a path between the two topologically inequivalent insulators that does not require any single-particle gap closing.

A dynamical mean-field theory (DMFT) study [34] extended the analysis to strongly correlated regimes: the EI is found to be robust against strong correlations and persists over an extended region of the (U, M) plane between the QSHI and the high-spin Mott insulator of Sec. 1.1, as summarised in Fig. 1.2a.

The most intriguing aspect of the DMFT phase diagram is the continuous character of the EI–MI transition. The existence of a continuous transition between the EI and the hs-MI implies that, as the EI boundary is approached from the Mott side, there must exist within the hs-MI an excitonic mode whose excitation energy goes to zero, i.e. a particle-hole bound state nearly degenerate with the ground state. This is a highly non-trivial requirement. The single-particle spectrum of the MI is dominated by lower and upper Hubbard bands separated by a charge gap of order U . A bound state between a particle in the upper Hubbard band and a hole in the lower one could have a vanishing excitation energy only if its binding energy were itself of order U . This would therefore imply a narrowing of the single-particle gap, which we only observe across the QSHI-to-EI transition. In contrast, the exciton softening on the MI side seems, to a large extent, unrelated to the Mott gap, which remains sizable, smooth and mono-

tonic across the transition. In other words, the transition between the EI and the MI is imperceptible in the evolution of the single-particle spectral gap, namely of the peaks of the imaginary part of the Green's function. One may wonder whether other features of the single-particle Green's function bear signatures of the exciton softening. In particular, since the Mott gap entails in-gap bands of Green's function zeros, it is conceivable that the latter bands are instead influenced by the transition, possibly in a manner similar to the bands of Green's function poles at the weak-coupling QSHI-to-EI transition. This is a suggestive conjecture that we shall investigate in this chapter.

1.3 The Green's function framework: poles, zeros, and topology

Before turning to the analysis of the excitonic instability, we introduce the Green's function framework that underpins the analysis discussed in the rest of this chapter. The purpose of this section is twofold. First, we review the distinction between poles and zeros of the single-particle Green's function, with particular emphasis on the physical meaning of Green's function zeros, including their possible connection to hidden quasiparticles [59, 60]. Second, we recall how the topology of an interacting system can be expressed in terms of the winding number of the single-particle Green's function, in which poles and zeros contribute on equal footing [47, 55].

1.3.1 Luttinger surfaces and hidden quasiparticles

Let us consider the one-body Green's function of an interacting electron system. In Matsubara frequencies $i\epsilon = (2n + 1)\pi T$, with $n \in \mathbb{Z}$, it can be written in terms of the self-energy $\Sigma(i\epsilon, \mathbf{k})$ as

$$G(i\epsilon, \mathbf{k}) = \frac{1}{i\epsilon - H_0(\mathbf{k}) - \Sigma(i\epsilon, \mathbf{k})}, \quad (1.17)$$

where $H_0(\mathbf{k})$ is the non-interacting Bloch Hamiltonian. The self-energy may be viewed as an effective, frequency-dependent one-body potential which encodes the effects of electronic correlations beyond the non-interacting Hamiltonian. It is useful to rewrite this expression in a form that makes contact with Fermi-liquid theory and, at the same time, allows one to treat conventional quasiparticle poles and Green's function zeros within a unified framework [47, 59, 60]. To this end, we introduce a quasiparticle Green's function G_* through

$$\begin{aligned} G(i\epsilon, \mathbf{k}) &= \frac{1}{i\epsilon - H_0(\mathbf{k}) - \Sigma(i\epsilon, \mathbf{k})} \\ &= \sqrt{Z(\epsilon, \mathbf{k})} \frac{1}{i\epsilon - H_*(\epsilon, \mathbf{k})} \sqrt{Z(\epsilon, \mathbf{k})} \\ &\equiv \sqrt{Z(\epsilon, \mathbf{k})} G_*(i\epsilon, \mathbf{k}) \sqrt{Z(\epsilon, \mathbf{k})} \end{aligned} \quad (1.18)$$

where we have introduced the positive semi-definite matrix

$$Z(\epsilon, \mathbf{k}) = Z(-\epsilon, \mathbf{k}) = \left(1 - \frac{\Sigma_2(i\epsilon, \mathbf{k})}{\epsilon}\right)^{-1} \quad (1.19)$$

in terms of

$$\begin{aligned} \Sigma_1(i\epsilon, \mathbf{k}) &= \frac{\Sigma(i\epsilon, \mathbf{k}) + \Sigma(i\epsilon, \mathbf{k})^\dagger}{2}, \\ \Sigma_2(i\epsilon, \mathbf{k}) &= \frac{\Sigma(i\epsilon, \mathbf{k}) - \Sigma(i\epsilon, \mathbf{k})^\dagger}{2i}, \end{aligned} \quad (1.20)$$

which are themselves Hermitian since $\Sigma(i\epsilon, \mathbf{k})^\dagger = \Sigma(-i\epsilon, \mathbf{k})$. The effective Hamiltonian $H_*(\epsilon, \mathbf{k})$ introduced in Eq. (1.18), which reads

$$\begin{aligned} H_*(\epsilon, \mathbf{k}) &= H_*(-\epsilon, \mathbf{k}) \\ &= \sqrt{Z(\epsilon, \mathbf{k})} (H_0(\mathbf{k}) + \Sigma_1(i\epsilon, \mathbf{k})) \sqrt{Z(\epsilon, \mathbf{k})}, \end{aligned} \quad (1.21)$$

is therefore also sometimes referred to as quasiparticle Hamiltonian within the scope of Fermi-liquid theory.

The representation in Eq. (1.18) separates the physical Green's function into two components: the quasiparticle propagator G_* , which determines the location of the low-energy quasiparticle poles, and the matrix Z , which controls their weight in the physical single-particle spectrum. As shown in Refs. [59, 60, 66], one can use $G_*(i\epsilon, \mathbf{k})$ to derive Landau's Fermi-liquid theory by following the same non-perturbative manipulations of the Bethe-Salpeter equation introduced by Luttinger and Nozières [67, 68]. This derivation requires that $Z(\epsilon, \mathbf{k})$ and $H_*(\epsilon, \mathbf{k})$ be analytic, at least to leading order, in ϵ within a finite interval around $\epsilon = 0$, and in $\mathbf{k}$ within a finite width shell around the quasiparticle Fermi surface. Within this formulation, the quasiparticle Fermi surface is defined as the surface in the Brillouin zone $\mathbf{k} = \mathbf{k}_{\text{FL}}$ where

$$\det(H_*(\epsilon \rightarrow 0, \mathbf{k}_{\text{FL}})) = 0. \quad (1.22)$$

Equivalently, the quasiparticle Fermi surface is the locus where $\det(G_*(i\epsilon, \mathbf{k}_{\text{FL}}))$ develops a pole at $\epsilon = 0$. Eq. (1.22) can be satisfied in two physically distinct ways, corresponding to two different types of quasiparticle.

- On a conventional Fermi surface $\mathbf{k}_{\text{FL}} \equiv \mathbf{k}_{\text{F}}$, the determinant in (1.22) vanishes because $\det(H_0(\mathbf{k}_{\text{F}}) + \Sigma_1(0, \mathbf{k}_{\text{F}}))$ in (1.21) goes to zero, while $\det(Z(0, \mathbf{k}_{\text{F}}))$ remains finite. In this case the pole of G_* at $\epsilon = 0$ also appears as a pole of the physical Green's function G , with finite spectral weight $Z(0, \mathbf{k}_{\text{F}}) < 1$.
- On a Luttinger surface, $\mathbf{k}_{\text{FL}} \equiv \mathbf{k}_{\text{L}}$, the determinant in Eq. (1.22) instead vanishes because $\det(Z(0, \mathbf{k}_{\text{L}}))$ tends to zero. This can occur when the self-energy develops a single pole at $\epsilon = 0$. Although $H_0(\mathbf{k}_{\text{L}}) + \Sigma_1(0, \mathbf{k}_{\text{L}})$ diverges, $Z(0, \mathbf{k}_{\text{L}})$ goes to 0 faster, compensating the divergence in such a way that $H_*(0, \mathbf{k}_{\text{L}})$ still has a zero eigenvalue. The quasiparticle pole is therefore present in G_* , but it manifests itself as a zero of the physical Green's function G because of the vanishing residue. Consequently, these quasiparticles are hidden, i.e. they are invisible in the single-particle spectral function.

The intriguing Luttinger surface scenario depicted above lies outside the original microscopic derivation of Landau's Fermi-liquid theory by Luttinger and Nozières [67, 68], who assumed the self-energy to be a regular, analytic function of frequency around $\epsilon = 0$. The assumption of analyticity required for $Z(\epsilon, \mathbf{k})$ and $H_*(\epsilon, \mathbf{k})$ only requires $\Sigma(i\epsilon, \mathbf{k})$ to be analytic at small but non-zero frequencies, while still being allowed to develop an isolated singularity at $\epsilon = 0$ [59, 60].

We conclude this section by providing a further argument in favor of the physical relevance of the quasiparticles associated with a Luttinger surface. The fact that they are hidden in the single-particle spectrum does not necessarily imply that they are incoherent excitations, and indeed they can be long lived and well-defined quasiparticles. After analytical continuation to real frequencies $i\epsilon \rightarrow \omega + i0^+$, the quasiparticle lifetime is controlled by the width $\Gamma(\omega, \mathbf{k})$ of the corresponding peak appearing in the spectral function

$$A(\omega, \mathbf{k}) = \frac{Z(\omega, \mathbf{k})}{\pi} \frac{\Gamma(\omega, \mathbf{k})}{\Theta(\omega, \mathbf{k})^2 + \Gamma(\omega, \mathbf{k})^2}, \quad (1.23)$$

where

$$\begin{aligned} Z(\omega, \mathbf{k}) &= \left(1 - \frac{\partial \text{Re}\Sigma(\omega, \mathbf{k})}{\partial \omega} \right)^{-1}, \\ \Theta(\omega, \mathbf{k}) &= Z(\omega, \mathbf{k}) (\omega - H_0(\mathbf{k}) - \text{Re}\Sigma(\omega, \mathbf{k})), \\ \Gamma(\omega, \mathbf{k}) &= -Z(\omega, \mathbf{k}) \text{Im}\Sigma(\omega, \mathbf{k}). \end{aligned} \quad (1.24)$$

The quasiparticle is sharp and infinitely long-lived if $\Gamma(\omega \rightarrow 0, \mathbf{k}) \rightarrow 0$ quadratically in ω . In an ordinary Fermi liquid, the imaginary part of the self-energy vanishes quadratically, $\text{Im}\Sigma(\omega, \mathbf{k}) \sim -\gamma(\mathbf{k})\omega^2$, while the quasiparticle residue stays finite, therefore $\Gamma(\omega, \mathbf{k}) \sim \omega^2$. On the other side, $\Gamma(\omega \rightarrow 0, \mathbf{k})$ can go to zero even when $\text{Im}\Sigma(0, \mathbf{k})$ remains finite, provided the residue compensates it by vanishing, $Z(\omega, \mathbf{k}) \sim \omega^2$. This is exactly the Luttinger surface scenario, where the self-energy is singular at $\omega = 0$ and the product $Z \text{Im}\Sigma$ still tends to zero and $\Gamma(\omega, \mathbf{k}) \rightarrow 0$ as expected for a Fermi liquid. We have thus depicted a broader formulation of Fermi-liquid theory, in which the emergence of low-energy quasiparticles is not tied exclusively to poles of the single-particle Green's function. Singular surfaces of the Green's function, whether associated with poles or zeros, can both serve as diagnostics of, possibly hidden, quasiparticles. Provided that the corresponding low-energy description remains analytic and supports a well-defined quasiparticle manifold, the response functions retain the characteristic Fermi-liquid form and are renormalized by Landau parameters. Within this framework, the low-energy collective dynamics are governed by quasiparticles even when the single-particle spectrum is gapped, as in a Mott insulating state. The existence of a Luttinger surface therefore does not contradict a Fermi-liquid description of the response functions, but rather extends its domain of applicability beyond systems characterized by a conventional quasiparticle Fermi surface [66].

1.3.2 The single-particle Green's function winding number

The analysis above has shown that, even in a strongly correlated insulator, a coherent single-particle-like description survives in the quasiparticle Hamiltonian $H_*(\epsilon, \mathbf{k})$, whose zero frequency spectrum encodes on the same footing the poles and the zeros of the physical Green's function. It is then natural to ask whether this same object also governs the *topological* character of the system, and in particular whether Green's function zeros are topologically relevant. Answering this question requires a notion of topological invariant that survives the loss of a non-interacting band picture. Indeed, the tools developed to characterize topological matter — Berry curvature, Chern numbers and their symmetry-protected refinements — were originally formulated for non-interacting Bloch Hamiltonians, where at each crystal momentum $\mathbf{k}$ one has direct access to the single-particle eigenstates and eigenvalues, and the topological indices are built from the occupied Bloch wavefunctions [6, 69, 70]. Strong correlations, however, defy a simple Bloch description: there is no longer a well-defined set of Bloch bands from which to construct these invariants, and one must rely on quantities that remain meaningful in the presence of interactions.

A natural route, available to all methods that grant access to the single-particle Green's function, such as DMFT and its cluster extensions, is to characterize the topology directly through the interacting Green's function. For a two dimensional insulator, the relevant invariant is the winding number of the map $(\epsilon, \mathbf{k}) \mapsto G(i\epsilon, \mathbf{k})$ [45, 46, 53, 70],

$$W[G] = \frac{1}{24\pi^2} \int d\epsilon d\mathbf{k} \epsilon_{\mu\nu\rho} \text{Tr} \left(G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\rho G^{-1} \right), \quad (1.25)$$

where $G \equiv G(i\epsilon, \mathbf{k})$, the indices μ, ν, ρ run over the three coordinates (ϵ, k_x, k_y) with $\partial_0 \equiv \partial_\epsilon$ and $\partial_{1,2} \equiv \partial_{k_{x,y}}$, $\epsilon_{\mu\nu\rho}$ is the antisymmetric tensor, and the frequency integral runs along the whole imaginary axis. The expression (1.25) is well defined whenever $G(i\epsilon, \mathbf{k})$ is an invertible matrix, i.e. for an insulator without a Luttinger surface, and it reduces to the first Chern number of the occupied bands once the interaction is switched off. When perturbation theory holds, $W[G]$ coincides with the zero temperature Hall conductance in units of e^2/h [36, 45–47].

The physical content of (1.25) becomes transparent in the quasiparticle representation of Eq. (1.18). The winding number is additive under matrix products, $W[G_1 G_2] = W[G_1] + W[G_2]$, and vanishes for any Hermitian matrix; consequently, the residue factors $\sqrt{Z(\epsilon, \mathbf{k})}$ in $G = \sqrt{Z} G_* \sqrt{Z}$ drop out entirely [36, 47],

$$W[G] = W[\sqrt{Z} G_* \sqrt{Z}] = W[G_*], \quad (1.26)$$

so that the invariant is controlled solely by the quasiparticle Green's function $G_*(i\epsilon, \mathbf{k}) = (i\epsilon - H_*(\epsilon, \mathbf{k}))^{-1}$. Since $H_*(\epsilon, \mathbf{k})$ is Hermitian and smooth and even in ϵ , the integrand of (1.25) can be recast as a total frequency derivative, whose only non-vanishing contribution comes from the step discontinuity at $\epsilon = 0$. The winding number then collapses onto the TKNN-like expression [6, 47, 63]

$$W[G] = \frac{i}{2\pi} \int d\mathbf{k} \epsilon_{ij} \sum_\alpha \theta(-\epsilon_\alpha(\mathbf{k})) \langle \partial_i \alpha(\mathbf{k}) | \partial_j \alpha(\mathbf{k}) \rangle, \quad (1.27)$$

namely the Chern number of the eigenstates $|\alpha(\mathbf{k})\rangle$ of the quasiparticle Hamiltonian $H_*(0, \mathbf{k})$ with negative eigenvalue $\epsilon_\alpha(\mathbf{k})$. Equivalently, $W[G]$ is the Chern number of the Hermitian matrix $-G_*(0, \mathbf{k})^{-1} = H_*(0, \mathbf{k})$, or of $-G(0, \mathbf{k})^{-1}$ [63]. Only the quasiparticle Hamiltonian at zero frequency thus enters the invariant, both in the perturbative and in the non-perturbative regime.

This result has a striking consequence in correlated insulators. Since (1.27) treats all eigenstates of $H_*(0, \mathbf{k})$ on the same footing, poles and zeros of the physical Green’s function contribute on equal footing to the topological invariant. In particular, in a Mott insulator the in-gap bands of Green’s function zeros can carry a non-trivial Chern number and thereby contribute to the topology of the system, even when the Hubbard bands are themselves topologically trivial [47, 55]. This will be central to the topological characterization of the correlated QSHI to MI transition addressed in this chapter.

1.4 The symmetric QSHI–MI transition

Equipped with the quasiparticle framework introduced in Sec. 1.3.1, we are now ready to study the interacting BHZ model. We begin, in this section, with the *symmetric* problem, i.e. in the absence of any spontaneous symmetry breaking (SSB): the leading instabilities identified in Sec. 1.1.3 are deliberately suppressed, so that the model evolves smoothly between the QSHI and MI. The excitonic insulator that intrudes between the two once SSB is allowed will be the subject of the following section. The full DMFT phase diagram in the (U, M) plane has been discussed at length in [34]; here we focus on how the transition is modified once two-sites non-local correlations are retained, and on the observation that bands of Green’s function zeros emerge already on the QSHI side of the transition. Unless otherwise stated, all results are obtained at inverse temperature $\beta = 50$, and we have checked their stability upon further lowering the temperature. We first introduce the numerical method, the dynamical cluster approximation, and then study the transition for both positive and negative coupling J .

1.4.1 Dynamical cluster approximation

As anticipated above, the bands of Green’s function zeros that are central to this chapter originate from poles of the self-energy, where $\Sigma(i\epsilon, \mathbf{k})$ diverges and drives $G(i\epsilon, \mathbf{k})$ to zero. Resolving these zeros as genuine *dispersive* bands in the Brillouin zone, and following their topological character across the QSHI–MI transition, therefore requires a self-energy that carries a non-trivial momentum dependence. This is information that DMFT [26] cannot provide: it approximates the self-energy as a purely local, momentum-independent quantity, $\Sigma(i\epsilon, \mathbf{k}) \simeq \Sigma(i\epsilon)$, so that the poles of the self-energy, and hence the associated bands of zeros, would be completely flat in momentum space.

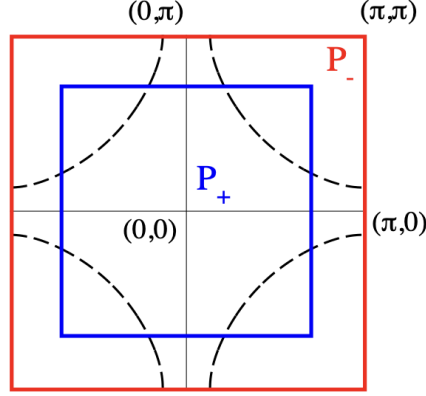


Figure 1.3: Partition of the square lattice Brillouin zone into the two DCA patches employed in this chapter, following Ref. [74]. The patch P_+ centered at $\Gamma = (0,0)$ and the patch P_- centered at $M = (\pi,\pi)$, the latter also enclosing the $X = (\pi,0)$ and $Y = (0,\pi)$ points. The self-energy is approximated as piecewise constant within each patch.

While DMFT captures the local correlation physics responsible for Mott localization, to endow the self-energy poles with dispersion — and, at the same time, to test the robustness of the excitonic instability against spatial fluctuations — we must turn to an extension of DMFT that retains momentum resolution. To this end we employ the dynamical cluster approximation (DCA) [32]. The DCA partitions the Brillouin zone into a finite set of patches and approximates the self-energy as a piecewise-constant function, $\Sigma(i\epsilon, \mathbf{k}) \simeq \Sigma(i\epsilon, \mathbf{K})$ for $\mathbf{k}$ in the patch $P(\mathbf{K})$ centered at the cluster momentum $\mathbf{K}$. The resulting problem maps onto a set of coupled quantum impurity models, solved self-consistently; we use the impurity solver of the TRIQS library [71] with a continuous-time quantum Monte Carlo algorithm based on the hybridization expansion of the partition function [72, 73].

In practice we employ two patches, centered at $\Gamma = (0,0)$ and $M = (\pi,\pi)$, with the M patch also enclosing the $X = (\pi,0)$ and $Y = (0,\pi)$ points, following the partition of Ref. [74] (see Fig. 1.3). While different choices for the shape of the patches can quantitatively change the results, we have explicitly checked that the conclusions discussed in the following are qualitatively robust against such variations. To reconstruct a smooth momentum dependence from the piecewise-constant DCA self-energy one can periodize either the self-energy or its inverse: the former works better at weak coupling, while the latter, known as cumulant periodization [75], is more suitable when the self-energy develops singularities in the Brillouin zone, as occurs near and inside the Mott insulator. We finally remark that, by inversion symmetry, the self-energy is diagonal at the high-symmetry points Γ and M ; the two-patch scheme therefore cannot resolve the off-diagonal components of $\Sigma(i\epsilon, \mathbf{k})$ that develop away from these points, whose inclusion would require a computationally prohibitive number of patches, but which have been shown not to play a crucial role in the QSHI–MI transition [76].

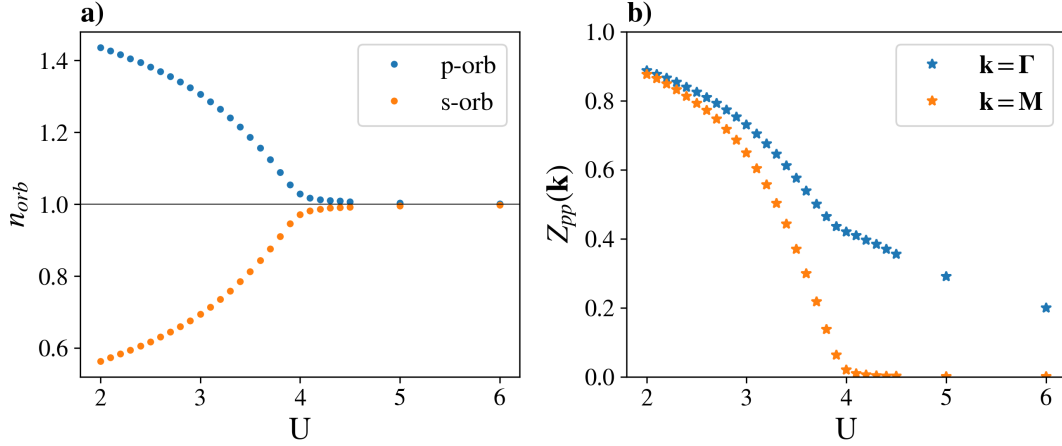


Figure 1.4: (a) Renormalization of the orbital occupations n_{orb} across the symmetric QSHI–MI transition, at fixed $M = 0.9$ and $J = U/4 > 0$. Deep in the MI phase the orbital polarization $n_p - n_s$ decays as $1/U^3$. (b) Quasiparticle residue $Z_{pp}(\mathbf{k}) = Z_{ss}(\mathbf{k})$ in the two patches, extracted from the imaginary part of the self-energy at the first Matsubara frequency. In the M patch it is strongly suppressed inside the MI, signalling the proximity to a self-energy pole, i.e. to a Luttinger surface. The change of concavity around $U \simeq 4$ marks the onset of the Mott insulating phase.

1.4.2 The $J > 0$ case

We set $V = U - 2J$, $J = U/4$, and study the symmetric QSHI–MI transition at fixed mass parameter $M = 0.9$. Since no symmetry is broken, spin $U(1)$ is preserved and the Green’s function is block-diagonal in the spin index; we may therefore restrict our following analysis to a single spin sector, with the 2×2 Green’s function given by the Dyson equation

$$\hat{G}(i\epsilon, \mathbf{k})^{-1} = i\epsilon - \hat{H}_0(\mathbf{k}) - \hat{\Sigma}(i\epsilon, \mathbf{k}), \quad (1.28)$$

with $\hat{H}_0(\mathbf{k})$ the corresponding 2×2 block of (1.4) and $\hat{\Sigma}(i\epsilon, \mathbf{k})$ the cluster self-energy. We recall that in single-site DMFT this transition is found to be first order [34]; one of our main results is that the inclusion of non-local correlations through DCA turns it into a continuous one.

In Fig. 1.4(a) we show the orbital occupations $n_{\text{orb}} = \langle n_{a\mathbf{R}} \rangle$ for $a = s, p$ as functions of U . At weak coupling the model is a QSHI adiabatically connected to the non-interacting one, and the main effect of the interaction is a renormalization of the on-site mass difference between the two orbitals, hence of the orbital polarization $n_p - n_s$. This renormalization can be encoded in an effective mass

$$M_{\text{eff}} = M + \frac{1}{4} \text{Tr}[\sigma_0 \otimes \tau_3 \hat{\Sigma}(i\epsilon = 0)], \quad (1.29)$$

where $\hat{\Sigma}(i\epsilon) = \frac{1}{2}[\hat{\Sigma}(i\epsilon, \Gamma) + \hat{\Sigma}(i\epsilon, M)]$ is the local (patch-averaged) self-energy. In the strong-coupling regime the system is instead a MI with nearly identical occupation of the two orbitals; deep in the Mott phase, second-order perturbation theory predicts

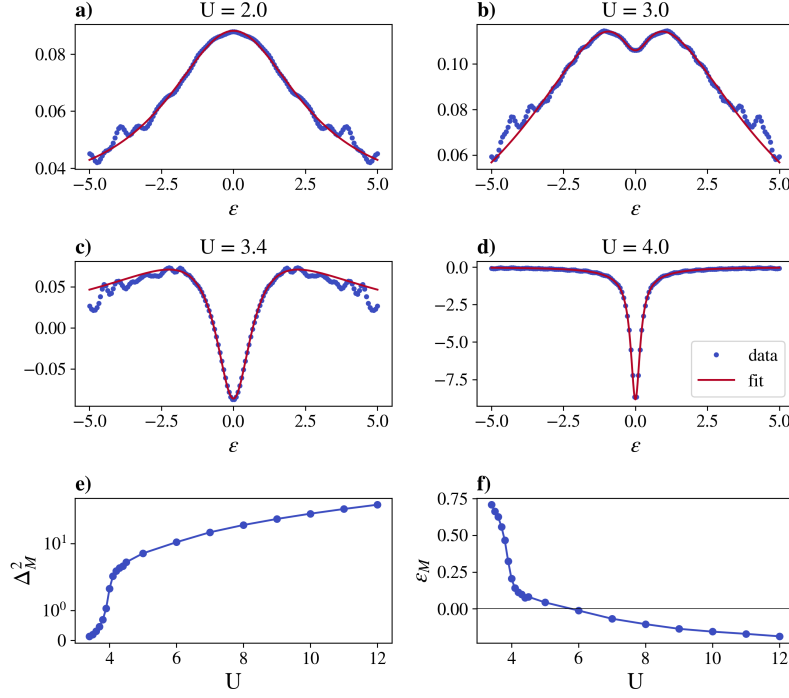


Figure 1.5: (a)–(d) Frequency dependence of $\Delta\hat{\Sigma}_{pp}(i\epsilon, M) = -\Delta\hat{\Sigma}_{ss}(i\epsilon, M)$ at fixed mass $M = 0.9$ for four values of U . For $U \gtrsim 3$ a narrow peak develops and becomes dominant as U increases; the fit (1.30) (red) reproduces the data well. (e),(f) Fit parameters of the narrow Lorentzian associated with the pole-like structure of the self-energy: its weight Δ_M^2 grows with U , while its position ϵ_M changes sign between $U = 5$ and $U = 6$, signalling a Dirac-type Luttinger surface at the high-symmetry point M .

that $n_p - n_s$ decays as $1/U^3$. Since $J > 0$ enforces Hund's rules, the two electrons localized on each site lock into a spin triplet with $S = 1$ and $S_z = \pm 1$, so that the resulting Mott state is the high-spin Mott insulator (hs-MI) anticipated in Sec. 1.1.

Fig. 1.4(b) shows the quasiparticle residue (1.19), here $Z_{pp}(\mathbf{k}) = Z_{ss}(\mathbf{k})$, in the two patches, computed from the imaginary part of the self-energy at the first Matsubara frequency $i\epsilon_1 = i\pi T$. At variance with single-site DMFT, none of these quantities displays a first-order discontinuity, which makes the transition harder to locate since the orbitals reach exact half-filling only as $U \rightarrow \infty$. Nonetheless, around $U \simeq 4$ we observe a change of concavity that we identify with the onset of the Mott insulating phase. Crucially, while Z_{pp} stays finite in the Γ patch, it is strongly suppressed in the M patch inside the MI: as discussed in Sec. 1.3.1, a vanishing residue signals the proximity to a pole of the self-energy at $\epsilon = 0$, i.e. to a Luttinger surface.

To better characterize the emergence of the Luttinger surface we inspect the frequency dependence of the self-energy. In Fig. 1.5 we plot $\Delta\hat{\Sigma}_{pp}(i\epsilon, \mathbf{k}) = \text{Re } \hat{\Sigma}_{pp}(i\epsilon, \mathbf{k}) - \hat{\Sigma}_{pp}^{\text{HF}}$, where $\hat{\Sigma}_{pp}^{\text{HF}}$ is the Hartree-Fock ($|\epsilon| \rightarrow \infty$) limit. In the M patch, where $\Delta\hat{\Sigma}_{pp}(i\epsilon, M) = -\Delta\hat{\Sigma}_{ss}(i\epsilon, M)$ by inversion symmetry, the curve looks like the difference between a broad Lorentzian and a narrower one that appears above $U = 3$ and grows with U , whereas in the Γ patch it is the sum of two Lorentzians. We therefore fit the data with

two Lorentzian contributions,

$$\Delta\hat{\Sigma}_{pp}(i\epsilon, \mathbf{k}) = -\frac{\alpha_{\mathbf{k}} \gamma_{\mathbf{k}}^2}{\epsilon^2 + \alpha_{\mathbf{k}}^2} - \frac{\epsilon_{\mathbf{k}} \Delta_{\mathbf{k}}^2}{\epsilon^2 + \epsilon_{\mathbf{k}}^2}, \quad (1.30)$$

the first being smooth, broad and qualitatively the same in the two patches, the second narrower and of opposite sign in the two patches. Each term is the real part, on the Matsubara axis, of a simple pole of the self-energy; we associate the narrow one with a pole-like structure that becomes dominant in the MI. Its fit parameters, shown in Figs. 1.5(e),(f), display two clear trends: the weight Δ_M^2 increases with U , making this contribution dominant in the Mott phase, while the pole position ϵ_M changes sign between $U = 5$ and $U = 6$.

This behavior is naturally rationalized by a simple toy model in which the effect of the broad Lorentzian is absorbed into the effective mass M_{eff} of (1.29), while only the singular Lorentzian is retained in the frequency-dependent part of the self-energy. The renormalized single-particle energies are then the eigenvalues of

$$\hat{R}(\mathbf{k}) = \hat{H}_0(\mathbf{k}) + \hat{\Sigma}_1(0, \mathbf{k}) = \hat{H}_0(\mathbf{k}) + \frac{\Delta^2}{\hat{H}_1(\mathbf{k})}, \quad (1.31)$$

where $\hat{H}_0(\mathbf{k})$ now carries the effective mass $M_{\text{eff}} < M$, and $\hat{H}_1(\mathbf{k})$ has the same form as (1.4) but with renormalized parameters. Since the self-energy diverges, and hence the Green’s function vanishes, where $\hat{H}_1(\mathbf{k})$ has a zero eigenvalue, the dispersive poles of $\hat{\Sigma}$ — i.e. the bands of Green’s function zeros — disperse as the eigenvalues of $-\hat{H}_1(\mathbf{k})$. The sign change of ϵ_M then corresponds to the renormalized mass M_1 of $\hat{H}_1(\mathbf{k})$ crossing $-2t_1$, that is, to a topological transition of the bands of zeros through a Dirac-type Luttinger surface, which here reduces to a single point at M . Because the two-patch scheme does not give access to the off-diagonal components of the self-energy away from the high-symmetry points, in what follows we add to $\hat{H}_1(\mathbf{k})$ a small $\lambda_1 = 0.2$ in order to correctly gap the Luttinger surfaces away from M , consistently with the finding [76] that such off-diagonal terms do not qualitatively affect the transition.

The topological content of these structures is best read off from the quasiparticle Hamiltonian $\hat{H}_*(\mathbf{k}) \equiv \hat{H}_*(0, \mathbf{k})$ of (1.21), whose spectrum, as established in Sec. 1.3.2, encodes on equal footing both the poles and the zeros of the physical Green’s function and determines the Green’s function winding number (1.27). In Fig. 1.6 we show the bands of $\hat{H}_*(\mathbf{k})$ across the transition, both in periodic (PBC) and open (OBC) boundary conditions, the latter in a slab geometry periodic along x and with $N_y = 200$ layers along y . At small interaction ($U = 2.0$) the only effect is the renormalization of the on-site mass difference: the system is adiabatically connected to the non-interacting QSHI and, in OBC, hosts genuine chiral edge states, i.e. gapless surface Green’s function poles. Increasing the interaction ($U = 3.4$), dispersive poles develop in the self-energy — equivalently, bands of Green’s function zeros appear — but without the bulk gap ever closing, so that the topological invariant is unchanged. Remarkably, in OBC there are now *three* pairs of chiral edge modes: two carried by Green’s function poles and one by zeros. This phase, in which topological bands of poles and zeros coexist, has

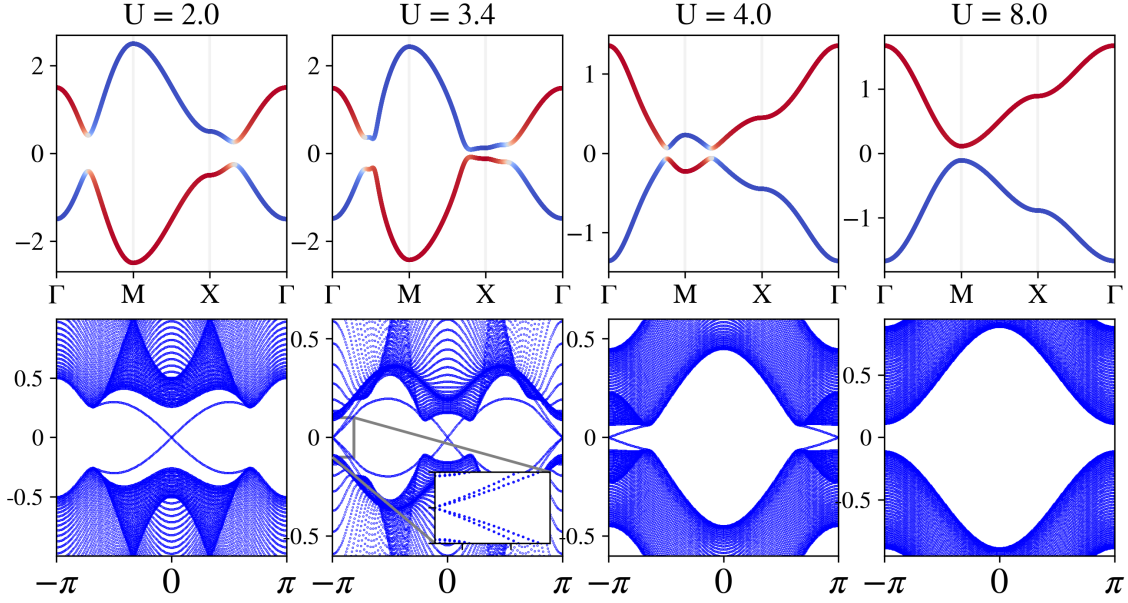


Figure 1.6: Bands of the quasiparticle Hamiltonian $\hat{H}_*(\mathbf{k}) = \hat{H}_*(0, \mathbf{k})$ obtained from the toy model (1.31) for four values of U , in periodic (upper panels, along $\Gamma \rightarrow M \rightarrow X \rightarrow \Gamma$) and open (lower panels) boundary conditions; the colour encodes the orbital character (s in blue, p in red). For $U = 2.0$ the system is adiabatically connected to the non-interacting QSHI. At $U = 3.4$ the topology is unchanged, but the OBC spectrum displays three pairs of chiral edge modes — two associated with Green's function poles and one with zeros (see inset). At $U = 4.0$ the model is a MI with topological in-gap bands of zeros, of winding number opposite to the QSHI, and a single pair of chiral edge zeros. At $U = 8.0$ the in-gap zeros have become topologically trivial and the system is smoothly connected to the atomic limit.

been dubbed a topological pseudogap insulator [61], by analogy with the pseudogap regime of weakly doped single-band Mott insulators.

Upon further increasing U ($U = 4.0$), the system undergoes a genuine topological transition driven by the bands of zeros: the gap of the quasiparticle Hamiltonian $\hat{H}_*(\mathbf{k})$ closes at the high-symmetry points X and Y — without any closing of the physical single-particle gap, which stays wide open — and beyond it the in-gap bands of zeros of the Mott insulator become topological, with winding numbers $W[G_\sigma]$ opposite to those of the QSHI (and not necessarily corresponding to well-defined Chern numbers C_σ [47]). Correspondingly, the OBC spectrum retains a single pair of chiral edge zeros. Finally, deep in the Mott phase ($U = 8.0$) also the bands of zeros become topologically trivial, touching in a Dirac-type fashion at the high-symmetry point M , and the system can be smoothly deformed into its atomic limit. We emphasize that the continuous character of the QSHI–MI transition survives upon lowering the temperature, which indicates that it is not a finite-temperature artefact but rather a consequence of the bands of Green's function zeros that appear already in the QSHI and evolve smoothly into the MI as U grows.

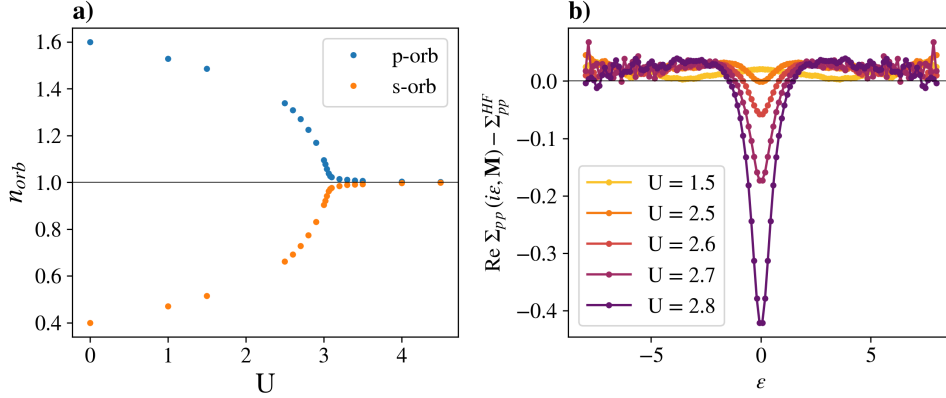


Figure 1.7: (a) Renormalization of the orbital occupations n_{orb} across the symmetric QSHI–MI transition for $J < 0$, at fixed $M = 1.0$. (b) Frequency dependence of $\Delta \hat{\Sigma}_{pp}(i\epsilon, M) = -\Delta \hat{\Sigma}_{ss}(i\epsilon, M)$ for several values of U below the onset of the MI ($U \simeq 3.1$). The phenomenology coincides with that of the $J > 0$ case of Figs. 1.4 and 1.5.

1.4.3 The $J < 0$ case

To probe the robustness of this picture against the nature of the Mott state, we repeat the analysis for $J < 0$, where, as discussed in Sec. 1.1, the local ground state is a non-magnetic inter-orbital singlet rather than a high-spin triplet. We choose $J = -U/2$, so that $V = 0$ and the model maps directly onto the bilayer construction of Slagle, You and Xu [51], in which the two layers are coupled solely through an antiferromagnetic exchange. As discussed in Sec. 1.1, we add the term (1.14) to favor the on-site spin-singlet configuration, thus stabilizing a low-spin Van Vleck Mott insulator; in the calculations we set $\delta J = U/16$.

Figure 1.7 shows the orbital occupations and the low-frequency self-energy across the transition at fixed $M = 1.0$. The phenomenology is identical to that for $J > 0$: the orbital polarization gradually diminishes, a pole-like structure emerges in the self-energy, and the QSHI–MI transition proceeds smoothly. The agreement between the $J > 0$ and $J < 0$ cases confirms that the emergence of bands of Green’s function zeros at the verge of the Mott transition is a universal feature of the correlated BHZ model, irrespective of the specific magnetic nature of the Mott insulator.

As we previously mentioned, the physics of the Mott phase in our model with $J < 0$ and $\delta J > 0$ should be similar to that in the bilayer model of Ref. [51]. However, in our case, the Mott transition is primarily driven by U , while in [51], it is driven by $|J| \gg U$. In both models, the Mott insulator is composed of singlets, which are on-site in our case and inter-layer in the bilayer model. Therefore, neither model can exhibit a finite, quantized spin-Hall conductance. Consequently, the high-spin MI at $J > 0$ should also have vanishing spin-Hall conductance. Furthermore, since the transition from the QSHI to the MI in [51] is accompanied by the vanishing of the spin and two-particle gaps, we suspect that the same happens in our model with $J < 0$ and

$\delta J > 0$. Additionally, since the transition appears to coincide with the point where the valence and conduction bands of zeros touch in a Dirac-like manner, we argue that gapless zeros are associated with gapless excitations.

1.5 The excitonic instability

Having characterized the symmetric transition, we now allow for spontaneous symmetry breaking and investigate the fate of the leading excitonic channel identified in Sec. 1.1.3. As anticipated in Sec. 1.2, both weak-coupling [33] and DMFT [34] studies have shown that an excitonic insulator (EI) could be stabilized upon raising the interaction in a QSHI. Here we revisit this instability within DCA.

1.5.1 The $J > 0$ case

We allow the system to develop a finite value of the excitonic order parameter (1.15); without loss of generality we work at $\phi = 0$ and monitor

$$P_1 = \langle \Psi_{\mathbf{R}}^\dagger \sigma_1 \otimes \tau_1 \Psi_{\mathbf{R}} \rangle, \quad (1.32)$$

calling excitonic insulator the phase characterized by $P_1 \neq 0$. As discussed in Sec. 1.1.3, a finite P_1 breaks inversion, time-reversal and the spin $U(1)$ symmetries that protect the topology of the QSHI, thus providing a path between topologically inequivalent insulators that does not require any single-particle gap closing.

In Fig. 1.8(a) we plot P_1 as a function of the interaction strength U for different values of M . Both the QSHI–EI and the EI–MI transitions seem to be second order within two-patch DCA; we recall that in single-site DMFT at $T = 0$ only the latter is so, while the QSHI–EI one is first order [34]. For smaller values of M , the range of stability of the EI shrinks. This could already be observed in DMFT, though there the EI survives down to $M \rightarrow 0$. On the contrary, the non-local correlations captured in DCA seem to prevent the stabilization of such a phase for $M \lesssim 0.6$, at least down to the lowest temperatures checked ($\beta = 150$). This scenario is further supported by the direct computation at $M = 0.5$ of the static and uniform susceptibility χ to a field coupled to the excitonic order parameter (1.32) [Fig. 1.8(b)]. In contrast to what we observe at larger M , e.g. $M = 1.5$ [Fig. 1.8(c)], there is no value of U such that the susceptibility diverges. However, we cannot exclude that, at lower temperatures than those we can access, the EI does appear.

We emphasize that the existence of an exciton condensate at finite temperature is a flaw of DCA, since long-range spatial correlations are treated in mean field. In fact, a finite order parameter (1.32) that breaks the continuous spin $U(1)$ symmetry is forbidden in two dimensions at any $T \neq 0$. Nonetheless, as noted in Sec. 1.1, the spin $U(1)$ symmetry is not exact in HgTe quantum wells; hence we expect that a phase transition separating

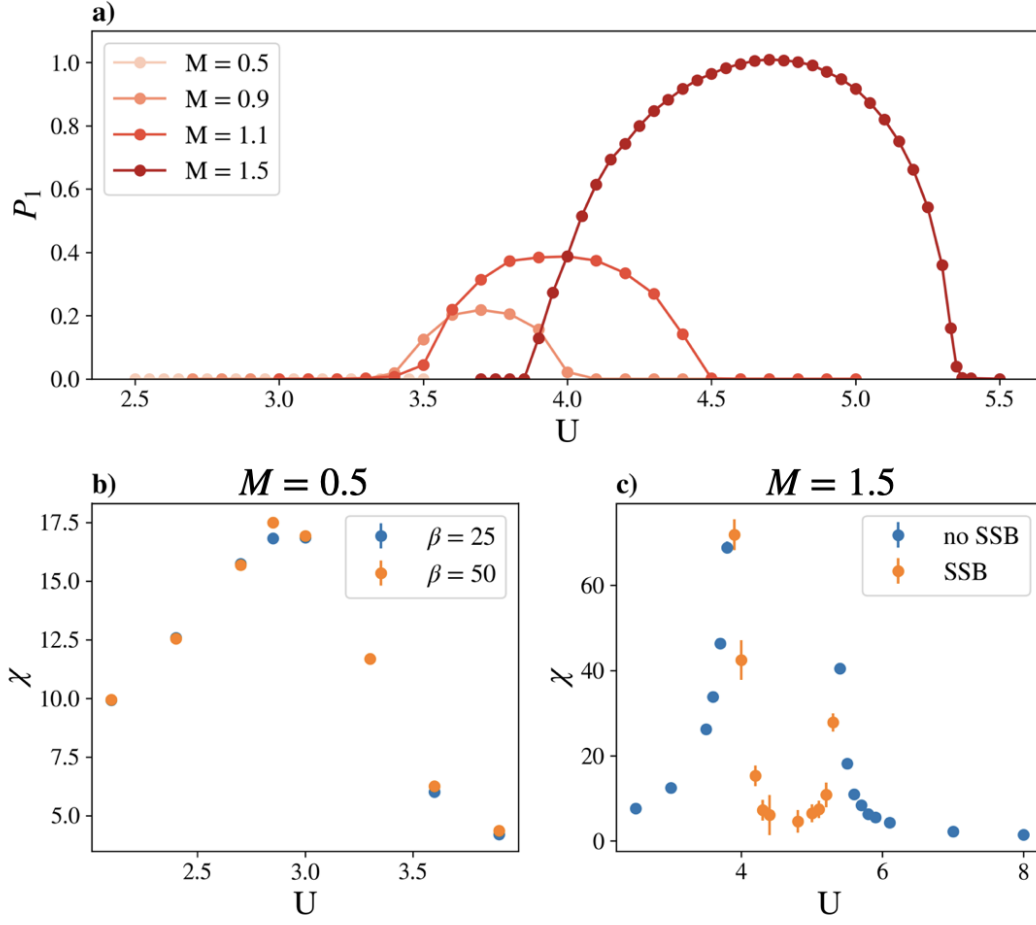


Figure 1.8: (a) Excitonic order parameter P_1 as a function of the interaction strength U for four different values of M , at $J = U/4 > 0$. As M decreases the bell-like dependence is strongly suppressed both in height and width, until for $M = 0.5$ no condensation appears; the results are stable down to the lowest temperature we checked, i.e. $\beta = 150$. (b) For $M = 0.5$, the susceptibility χ to an external field coupled to the excitonic order parameter never diverges, corroborating the absence of condensation; there is no substantial difference between $\beta = 25$ and $\beta = 50$, further suggesting this is not a temperature consequence. (c) For $M = 1.5$ the susceptibility diverges at the phase boundaries of the EI.

a low-temperature phase with finite order parameter from a high-temperature phase with vanishing order parameter could in reality exist.

1.5.2 The $J < 0$ case

For $J < 0$ the EI is instead characterized by the order parameter (1.16),

$$P_2 = \langle \Psi_{\mathbf{R}}^\dagger \sigma_0 \otimes \tau_1 \Psi_{\mathbf{R}} \rangle, \quad (1.33)$$

which breaks inversion but preserves time-reversal. Figure 1.9 shows P_2 as a function of U at $M = 1.0$. The EI is again found to intrude between the QSHI and the (low-spin) Mott insulator, but with one notable difference with respect to the $J > 0$ case: the QSHI–EI transition now appears to be first order, while the EI–MI transition remains continuous. As for $J > 0$, we are unable to stabilize the EI at small values of M , down to the lowest accessible temperatures.

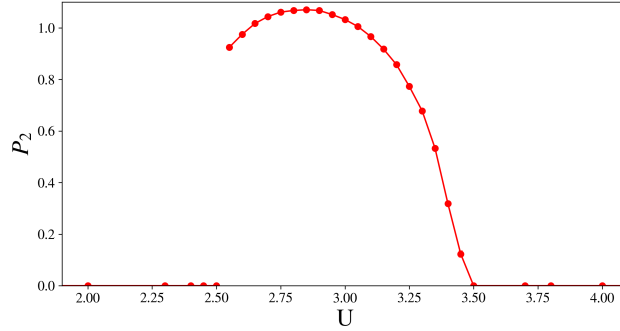


Figure 1.9: Excitonic order parameter P_2 for $J < 0$ at $M = 1.0$. At variance with the $J > 0$ case, the QSHI–EI transition is first order, while the EI–MI transition is still continuous.

1.5.3 Excitonic instability of the Mott insulator and the quasiparticle scenario

We now address the most intriguing aspect of the phase diagram, focusing for definiteness on the $J > 0$ case: the microscopic nature of the excitons that soften at the EI–MI boundary. While the QSHI–EI instability can be understood in conventional terms as the softening of an exciton bound state between the valence and conduction bands as the single-particle gap shrinks, this picture is untenable at the EI–MI transition. In the MI the single-particle gap is large, which would seemingly preclude the formation of a particle-hole bound state capable of softening upon approaching the transition. As anticipated in Sec. 1.2, this observation prompts the conjecture that, in the MI, the relevant excitons are bound states between the valence and conduction bands of Green's function *zeros*, rather than between the lower and upper Hubbard bands.

This scenario is rooted in the quasiparticle picture of Sec. 1.3.1, and comes about spontaneously once we notice that a Luttinger surface may host Landau's quasiparticles [59], similarly to a Fermi surface. These quasiparticles cannot transport charge if the system is a true MI: one should imagine that their motion is cancelled by a charge backflow,

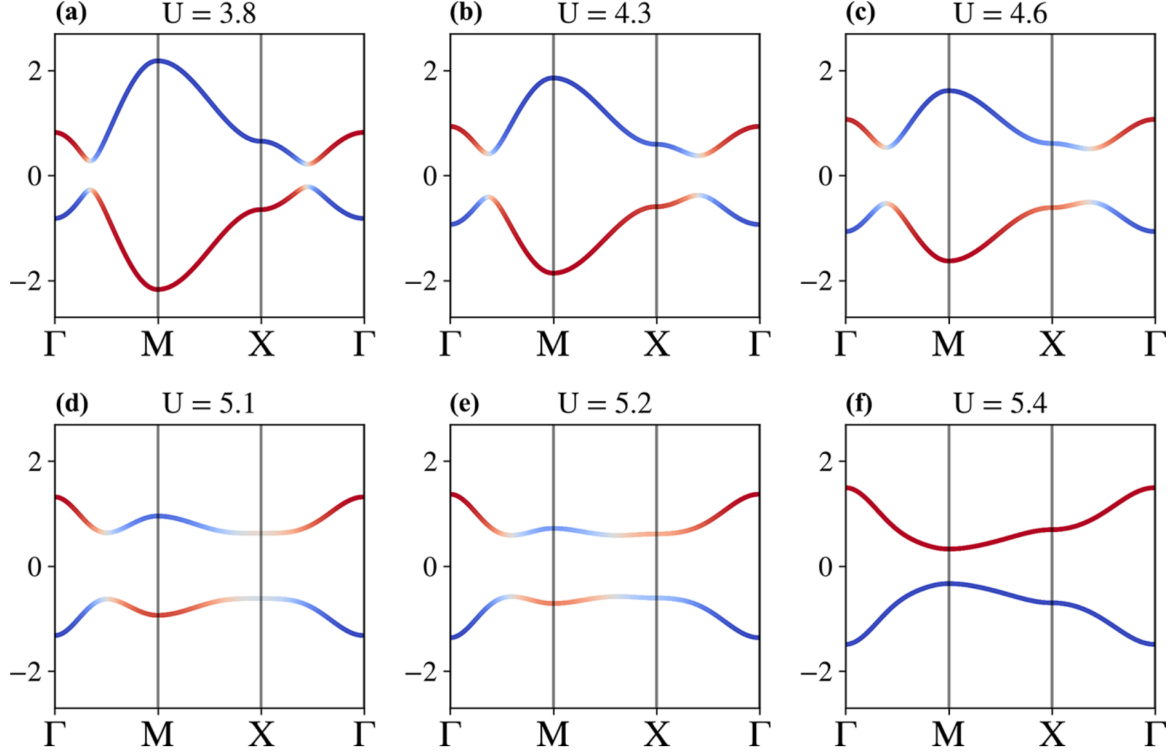


Figure 1.10: Bands of the quasiparticle Hamiltonian $\hat{H}_*(\mathbf{k})$ across the QSHI–EI–MI transitions at $M = 1.5$ and $J > 0$; the colour encodes the orbital character (s in blue, p in red). Panel (a) is the QSHI; in (b)–(e) the system is an EI with $P_1 \neq 0$, which breaks inversion so that the orbital character at the high-symmetry points is no longer well defined; in (f) the quasiparticle bands closely resemble the dispersive Green’s function zeros of the Mott insulator. The bands evolve smoothly across both transitions.

so that no net longitudinal current flows in an electric field. They are nonetheless not neutral in the strict sense, as they can still transport entropy and spin, and even experience a Lorentz force in a magnetic field [58, 60, 61]. In the present model these dressed quasiparticles carry an additional quantum number, the parity, which both allows a hybridization gap to open and permits the formation of bound states between opposite-parity quasiparticle and quasihole excitations. Since these anomalous quasiparticles are intimately tied to the in-gap bands of Green’s function zeros [47, 55, 57], their bound states can be viewed precisely as bound states between the valence and conduction bands of zeros. Consistently, a Mott insulator with a Luttinger surface has been shown to display an odd-parity exciton susceptibility that is power-law in temperature, suggestive of gapless opposite-parity quasiparticles [61].

To substantiate this interpretation we again turn to the quasiparticle Hamiltonian $\hat{H}_*(\mathbf{k})$ of (1.21). Figure 1.10 shows its bands across the two transitions at $M = 1.5$; denoting by $U_{*1} \simeq 3.9$ and $U_{*2} \simeq 5.3$ the QSHI–EI and EI–MI critical couplings, the system is a QSHI for $U < U_{*1}$, an EI with $P_1 \neq 0$ for $U_{*1} < U < U_{*2}$, and a Mott insulator for $U > U_{*2}$. In the EI the broken inversion symmetry is manifest in the loss of a well-defined orbital character at the high-symmetry points, and for $U > U_{*2}$ the

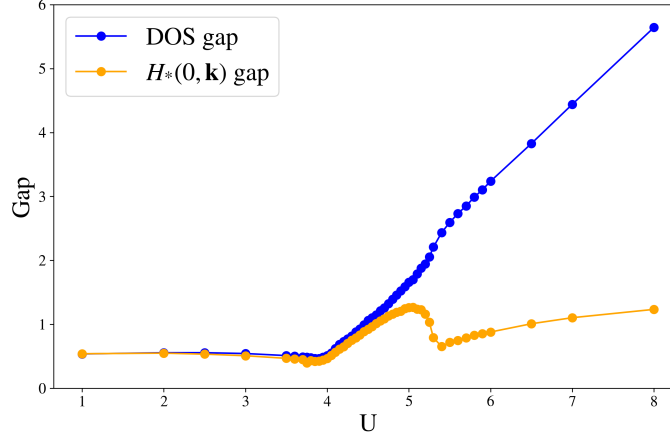


Figure 1.11: Comparison between the quasiparticle gap of $\hat{H}_*(\mathbf{k})$ and the single-particle gap extracted from the density of states (DOS) across the QSHI–EI–MI transitions. The condensation of excitons increases the quasiparticle gap on entering the EI from both sides, whereas the single-particle gap decreases at the EI–MI boundary. The point at which the two gaps start to deviate marks the onset of the bands of zeros.

quasiparticle bands come to closely resemble the dispersive Green's function zeros of the Mott insulator. Remarkably, the quasiparticle bands evolve *smoothly* across both transitions, despite the very different nature of the two phases — a clear advantage of the quasiparticle description of Sec. 1.3.1.

The strongest evidence for our scenario is provided by Fig. 1.11, where we compare the quasiparticle gap, i.e. the gap of $\hat{H}_*(\mathbf{k})$, with the single-particle Mott gap extracted from the density of states. In a conventional insulator, exciton condensation raises the single-particle gap, because it generates an additional level repulsion between valence and conduction bands. This is indeed what happens at the QSHI–EI transition, but not at the EI–MI one, where the single-particle gap keeps growing. The quasiparticle gap, on the contrary, behaves as expected of a conventional excitonic insulator: it grows upon entering the EI from both the QSHI and the Mott sides. We further note that single-particle and quasiparticle gaps are practically the same on increasing U up to around the value at which P_1 reaches a maximum, see Fig. 1.8(a). Above that value, while the single-particle gap keeps growing with U , the quasiparticle one first decreases up to the Mott transition and then rises again, though remaining much smaller than the single-particle gap. The point at which the two gaps start to deviate from each other is also the one at which the bands of zeros come into play, which thus occurs already inside the EI. Indeed, looking at the low-frequency behaviour of the self-energy in the EI we can still identify a structure made up of two Lorentzians, as the one we discussed in Fig. 1.5.

The remarkable behavior reported in Fig. 1.11 aligns with a scenario in which the exciton that softens in the Mott insulator is formed between the valence and conduction bands of zeros, rather than between the lower and upper Hubbard bands. If interpreted literally, this implies that the bands of zeros are linked to exotic valence and

conduction quasiparticles that carry spin, entropy, and parity but not charge. While these quasiparticles are invisible in the single-particle spectrum, they could manifest in the particle-hole spectrum, specifically in the triplet channel that is odd under parity. It is possible that not all the spectral weight in this channel is accounted for by the bound state, but a small portion may remain in a continuum, indicating the underlying quasiparticle constituents of the excitons.

1.6 Conclusions

In this chapter we have analyzed the interaction-driven transitions in a BHZ model for a quantum spin Hall insulator (QSHI) within the dynamical cluster approximation (DCA), which retains the non-local correlations needed to endow the poles of the self-energy, and hence the associated bands of Green's function zeros, with a genuine dispersion.

In the absence of symmetry breaking, bands of Green's function zeros emerge already in the QSHI, where they give rise to a "topological pseudogap insulator" [61] that, in open boundary conditions, hosts two chiral branches of edge poles and one of zeros, without altering the spin Chern number of the weakly correlated state and thus without requiring any topological transition. The topological bands of zeros survive inside the Mott insulator (MI), where they sustain edge zeros in open boundary conditions, until at a critical interaction strength they touch in a Dirac-like fashion at the high-symmetry point M , become trivial, and the insulator can be smoothly deformed into its atomic limit. We emphasize that the similarities observed in the two cases with $J > 0$ and $J < 0$, and the affinity of the latter case with the model studied in [51], suggest that the Mott phases that we find do not have spin-Hall conductance, despite exhibiting a finite winding number for not too large U . Consequently, we expect that some particle-hole or particle-particle gap should close at the transition, in analogy with [51].

Once symmetry breaking is allowed, a non-topological excitonic insulator intrudes between the QSHI and the MI [34]. The two-patch DCA does not recover the magnetic instability expected in the Mott phase, a known limitation of the cluster size we can afford [77]. To ensure that our conclusions are not an artifact of this approximation, we have also studied the inverted-exchange model that stabilizes a Van Vleck paramagnetic MI, finding the same qualitative behaviour. Most importantly, the analysis of the quasiparticle Hamiltonian provides evidence that the exciton softening at the boundary with the MI is a bound state between the valence and conduction bands of Green's function zeros, rather than between the lower and upper Hubbard bands. The existence of this buffer phase serves as an effective bridge between the QSHI and the MI without crossing a metallic point. It appears somewhat surprising that such an intermediate phase does not emerge in the bilayer model studied by Slagle, You, and Xu [51], considering that when we prevent exciton condensation, we observe a similar

behavior as in [51].

The depicted scenario of an excitonic insulator intruding between a topological and a Mott insulator might be realized in topological materials whose interaction strength can be tuned across a Mott transition. The best-known topological insulators are likely too weakly correlated to be favourable candidates, whereas topological Kondo insulators [78] could be more promising, provided a negative chemical pressure pushed them towards Mott localization. Alternatively, since the inversion- and time-reversal breaking excitonic insulator is magnetoelectric [33, 34], magnetoelectric insulators that can be turned topological or Mott by external means represent an interesting avenue worth exploring.

CHAPTER 2

Fermi liquid corrections to the intrinsic anomalous Hall conductivity of topological metals

In this chapter, we show that the intrinsic anomalous Hall conductivity of an interacting topological metal is contributed not only by the quasiparticle Berry phase, but receives Fermi liquid corrections from the residual interactions among them. These corrections, alike the Berry-phase term itself, originate entirely from the Fermi surface. This chapter is based on Ref. [36].

Introduction

In the previous chapter we have seen that, even in the presence of interactions, the topology of the two-dimensional ground state is encoded in the winding number $W[G]$ of the single-particle Green's function. For non-interacting electrons $W[G]$ coincides with the Hall conductance in units of $e^2/2\pi\hbar$, thus a finite winding number implies a finite Hall response. Strikingly, $W[G]$ can remain quantised and non-trivial even across the transition into a Mott insulator, where it is carried by the in-gap bands of Green's function zeros [30, 47, 55], while the Hall conductance may well vanish. Strong interactions, in particular beyond the perturbative regime, thus open a genuine discrepancy between the topological invariant $W[G]$ and the physically measured Hall conductance. Here, we consider the complementary case of a topological metal, where the intrinsic anomalous Hall conductivity (AHC) is in general non-quantised, and we show how it acquires corrections from the residual interactions among the quasiparticles.

The anomalous Hall effect, the appearance of a transverse conductivity in the absence of an external magnetic field, has a long and rich history that dates back to the work of Karplus and Luttinger [79]. It is customary to separate its *extrinsic* contributions, due to skew scattering and side jump off impurities, from the *intrinsic* one, which is a property of the perfect crystal alone [80]. For non-interacting electrons the intrinsic AHC is a purely geometric quantity: it is the Brillouin zone integral of the Berry curvature of the occupied Bloch bands, the very same TKNN integral that, in an insulator, quantises the Hall conductance [6]. In a metal the integral is cut off at the Fermi

level and the result is no longer quantised. Haldane showed [35] that this integral can nonetheless be recast, through an integration by parts, as a Fermi surface integral of the Berry phase accumulated by the quasiparticles, as later confirmed in ab-initio calculations [81], and in agreement with the spirit of Landau’s theory of Fermi liquids [3]. However, Haldane’s work leaves open an important issue that we now discuss. Landau’s energy functional for the quasiparticles comprises both a quasiparticle Hamiltonian $\hat{H}_*(\mathbf{k})$ and a residual interaction encoded in the Landau f -parameters that we write as a tensor $\hat{f}(\mathbf{k}, \mathbf{k}')$ in band space. It is tempting to assume that the quasiparticle topology is contained entirely in $\hat{H}_*(\mathbf{k})$ and its Bloch eigenstates $|\psi_n(\mathbf{k})\rangle$, so that the AHC follows from the Berry curvature of these states exactly as for non-interacting electrons. There is, however, growing evidence that this reasonable looking choice is incorrect [47, 82, 83]: because the quasiparticles do interact, the bare Berry curvature of the $|\psi_n(\mathbf{k})\rangle$ does not by itself yield the anomalous Hall conductivity, which acquires additional vertex corrections. This naturally raises the question of whether such corrections are compatible with Landau’s Fermi liquid theory. This is precisely the aim of the present chapter.

The chapter is organised as follows. In Sec. 2.1 we introduce the multi-band formalism of Landau’s Fermi liquid theory and we derive the Hall conductivity tensor, including the Fermi liquid corrections due to the residual interactions between the quasiparticles. In Sec. 2.2 we specialize our discussion to a model topological metal with broken time-reversal symmetry, where we can explicitly verify that the corrections to the anomalous Hall conductivity stem solely from the quasiparticle Fermi surface. In Sec. 2.3 we discuss the implications of our results, with emphasis on correlated ferromagnetic metals.

2.1 Hall conductivity within Landau’s Fermi liquid theory

We consider a periodic system of interacting electrons, thus in absence of impurities and their extrinsic contributions to the anomalous Hall effect [80], at sufficiently low temperature to safely discard any quasiparticle decay rate. We account for the general case of many bands crossing the chemical potential that can be described within Landau’s Fermi liquid theory. We shall deal with this theory following an early observation by Leggett [84]. Indeed, one may realise [66, 84] that Landau’s Fermi liquid theory basically shows [67, 68] that the low-frequency, long-wavelength and low-temperature response functions of the physical electrons correspond to those of a system of interacting quasiparticles treated by the Hartree-Fock (HF) plus the random phase (RPA) approximations. This correspondence can be drawn only in the limits where one can make use of the Ward-Takahashi identities [67, 68], therefore only in connection with densities associated to conserved quantities and their corresponding currents, and either in the q -limit, i.e. the transferred frequency vanishing faster than the transferred momentum, or in the opposite ω -limit depending on the specific response function. A complete and rigorous derivation, which generalises the work of Nozières and Luttinger

to the multiband case, can be found in Ref. [36] and we shall not reproduce it here. We thus consider quasiparticles described by an interacting Hamiltonian, setting $\hbar = 1$ hereafter,

$$H_{\text{qp}} = H_0 + H_{\text{int}}, \quad H_0 = \sum_{\mathbf{k}} \sum_{\alpha\beta} c_{\alpha\mathbf{k}}^\dagger H_{0\alpha\beta}(\mathbf{k}) c_{\beta\mathbf{k}}, \quad (2.1)$$

where H_0 is a one-body term, e.g. a tight-binding Hamiltonian, $c_{\alpha\mathbf{k}}$ annihilates a quasiparticle with momentum $\mathbf{k}$ in the state α (which collects both the band index and the spin σ), and H_{int} is the interaction, which we need not specify. Within HF one replaces (2.1) by the non-interacting Hamiltonian

$$\hat{H}_*(\mathbf{k}) = \hat{H}_0(\mathbf{k}) + \hat{\Sigma}_{\text{HF}}[\mathbf{k}, \hat{G}_*], \quad (2.2)$$

in which $\hat{\Sigma}_{\text{HF}}$ retains only the Hartree and Fock diagrams of the self-energy functional, and

$$\hat{G}_*(i\epsilon, \mathbf{k}) = \frac{1}{i\epsilon - \hat{H}_*(\mathbf{k})}. \quad (2.3)$$

is the HF Green's function in Matsubara frequencies. Eq. (2.2) is in reality a self-consistency equation, whose solution provides $\hat{G}_*(i\epsilon, \mathbf{k})$. RPA is a symmetry-conserving scheme consistent with HF [66]: it amounts to computing the response functions with the Green's function (2.3) and with the irreducible scattering vertex in the particle-hole channel defined as

$$\frac{\delta \hat{\Sigma}_{\text{HF}}[\mathbf{k}, \hat{G}_*]}{\delta \hat{G}_*(i\epsilon, \mathbf{k}')} = \hat{f}(\mathbf{k}, \mathbf{k}'), \quad (2.4)$$

which provides the definition of the Landau f -parameter tensor. Accordingly, the quasiparticle energies $\varepsilon_\ell(\mathbf{k})$ and eigenstates $|\psi_\ell(\mathbf{k})\rangle$ — where roman letters distinguish them from the greek labels of the original basis — follow from diagonalising

$$H_{*\alpha\beta}(\mathbf{k}) = H_{0\alpha\beta}(\mathbf{k}) + \frac{T}{V} \sum_{\mathbf{k}'\mu\nu} \sum_{\epsilon} e^{i\epsilon 0^+} f_{\alpha\nu, \mu\beta}(\mathbf{k}, \mathbf{k}') G_{*\mu\nu}(i\epsilon, \mathbf{k}'), \quad (2.5)$$

where V is the volume and the expectation values, to be determined self-consistently, are over the HF ground state. The diagonalisation is accomplished by a unitary transformation $\hat{U}(\mathbf{k})$,

$$\hat{U}(\mathbf{k})^\dagger \hat{H}_*(\mathbf{k}) \hat{U}(\mathbf{k}) = \hat{\varepsilon}_*(\mathbf{k}), \quad (2.6)$$

with $\hat{\varepsilon}_*(\mathbf{k})$ the diagonal matrix of elements $\varepsilon_\ell(\mathbf{k})$. We shall refer to the basis that diagonalises $\hat{H}_*(\mathbf{k})$ as the HF basis.

Before delving into the analysis of the Hall conductivity, we briefly recall the main results of Landau's Fermi liquid theory: namely how to derive the q - and ω -limits of the response functions of the physical electrons from those of the quasiparticles, using the formal manipulations of the Bethe-Salpeter equation.

2.1.1 Fermi-liquid response functions

The Bethe-Salpeter equation for the reducible particle-hole vertex in terms of the f -parameters reads

$$\Gamma_{\ell m, np}(\mathbf{k}, \mathbf{k}'; i\omega, \mathbf{q}) = f_{\ell m, np}(\mathbf{k}, \mathbf{k}') + \frac{1}{V} \sum_{\mathbf{p}} \sum_{qs} f_{\ell s, qp}(\mathbf{k}, \mathbf{p}) R_{sq}(\mathbf{p}; i\omega, \mathbf{q}) \Gamma_{qm, ns}(\mathbf{p}, \mathbf{k}'; i\omega, \mathbf{q}), \quad (2.7)$$

where ω and $\mathbf{q}$ are, respectively, the frequency and momentum transferred in the particle-hole channel, and the kernel is

$$R_{sq}(\mathbf{p}; i\omega, \mathbf{q}) = T \sum_{\epsilon} \frac{1}{i\epsilon + i\omega - \varepsilon_q(\mathbf{p} + \mathbf{q})} \frac{1}{i\epsilon - \varepsilon_s(\mathbf{p})} = \frac{f(\varepsilon_s(\mathbf{p})) - f(\varepsilon_q(\mathbf{p} + \mathbf{q}))}{i\omega + \varepsilon_s(\mathbf{p}) - \varepsilon_q(\mathbf{p} + \mathbf{q})}, \quad (2.8)$$

where we have explicitly performed the Matsubara sum, with $f(x)$ being the Fermi distribution function, not to be confused with the Landau parameters $f_{\ell m, np}$, which carry indices. In compact notation, with $\odot$ denoting the sum over internal indices and momenta, Eq. (2.7) reads

$$\Gamma = f + f \odot R \odot \Gamma = f + \Gamma \odot R \odot f. \quad (2.9)$$

We now perform a series of formal and exact manipulations of (2.9), analogous to those used by Nozières and Luttinger to derive Landau's theory [67, 68], which we report explicitly since they may be unfamiliar. From (2.9) we get

$$f = \Gamma \odot (1 + R \odot \Gamma)^{-1}. \quad (2.10)$$

Taking the q -limit of (2.9), i.e. sending first $\omega \rightarrow 0$ and then $\mathbf{q} \rightarrow 0$,

$$\Gamma^q = f + \Gamma^q \odot R^q \odot f = f + f \odot R^q \odot \Gamma^q, \quad (2.11)$$

one finds

$$f = (1 + \Gamma^q \odot R^q)^{-1} \odot \Gamma^q. \quad (2.12)$$

The irreducible vertex f does not include the kernel R , i.e., a particle line and a hole one differing by frequency $i\omega$ and momentum $\mathbf{q}$, and therefore, cannot have any singularity in that channel: thus $f \equiv f^\omega \equiv f^{\mathbf{q}}$.

Comparing now (2.10) with (2.12) yields

$$\Gamma \odot (1 + R \odot \Gamma)^{-1} = (1 + \Gamma^q \odot R^q)^{-1} \odot \Gamma^q, \quad (2.13)$$

hence

$$(1 + \Gamma^q \odot R^q) \odot \Gamma = \Gamma^q \odot (1 + R \odot \Gamma), \quad (2.14)$$

and therefore

$$\Gamma = \Gamma^q + \Gamma^q \odot (R - R^q) \odot \Gamma = \Gamma^q + \Gamma \odot (R - R^q) \odot \Gamma^q. \quad (2.15)$$

On the other hand, from (2.15) it follows that

$$\Gamma^q = \Gamma \odot [1 + (R - R^q) \odot \Gamma]^{-1}, \quad (2.16)$$

and thus

$$\begin{aligned} 1 + R^q \odot \Gamma^q &= 1 + R^q \odot \Gamma \odot [1 + (R - R^q) \odot \Gamma]^{-1} \\ &= [1 + (R - R^q) \odot \Gamma] \odot [1 + (R - R^q) \odot \Gamma]^{-1} \\ &\quad + R^q \odot \Gamma \odot [1 + (R - R^q) \odot \Gamma]^{-1} \\ &= (1 + R \odot \Gamma) \odot [1 + (R - R^q) \odot \Gamma]^{-1}. \end{aligned} \quad (2.17)$$

The dressed current vertex J is obtained from the bare one J_0 , which we actually do not know, through the Bethe-Salpeter equation

$$J = J_0 + J_0 \odot R \odot \Gamma = J_0 + \Gamma \odot R \odot J_0, \quad (2.18)$$

whose q -limit is

$$J^q = J_0 + J_0 \odot R^q \odot \Gamma^q. \quad (2.19)$$

As before, we use (2.18) to solve for the unknown J_0 ,

$$J_0 = J \odot (1 + R \odot \Gamma)^{-1}, \quad (2.20)$$

and, taking the q -limit as well and making use of (2.17),

$$\begin{aligned} J_0 &= J^q \odot (1 + R^q \odot \Gamma^q)^{-1} \\ &= J^q \odot [1 + (R - R^q) \odot \Gamma] \odot (1 + R \odot \Gamma)^{-1} \\ &= (1 + \Gamma \odot R)^{-1} \odot [1 + \Gamma \odot (R - R^q)] \odot J^q, \end{aligned} \quad (2.21)$$

which, compared with (2.20), leads to

$$J = J^q + J^q \odot (R - R^q) \odot \Gamma = J^q + \Gamma \odot (R - R^q) \odot J^q. \quad (2.22)$$

The current-current response function is defined, in short notation, through

$$\chi_{JJ} \equiv \text{Tr}(J \odot R \odot J_0) = \text{Tr}(J_0 \odot R \odot J), \quad (2.23)$$

whose q -limit is therefore $\chi^q = \text{Tr}(J^q \odot R^q \odot J_0)$. Making use of (2.18) and (2.22) we can write

$$\begin{aligned} \chi_{JJ} &= \chi^q + \text{Tr}(J \odot R \odot J_0) - \text{Tr}(J^q \odot R^q \odot J_0) \\ &= \chi^q + \text{Tr}(J^q \odot (R - R^q) \odot J_0) + \text{Tr}(J^q \odot (R - R^q) \odot \Gamma \odot R \odot J_0) \\ &= \chi^q + \text{Tr}(J^q \odot \Delta \odot J) \\ &= \chi^q + \text{Tr}(J^q \odot \Delta \odot J^q) + \text{Tr}(J^q \odot \Delta \odot \Gamma \odot \Delta \odot J^q), \end{aligned} \quad (2.24)$$

where we have defined $\Delta = R - R^q$. We can now invoke symmetries and the Ward-Takahashi identities. Gauge symmetry entails that χ^q must precisely cancel the diamagnetic term D , which we likewise do not know,¹ while the Ward-Takahashi identities fix the q -limit of the current vertex to $J^q(\mathbf{k}) \equiv \nabla_{\mathbf{k}} \hat{H}_*(\mathbf{k})$ [67, 68]. Correspondingly, the component $\sigma_{ab}(i\omega, \mathbf{q})$ of the conductivity tensor follows from the Kubo formula which, with these substitutions, reads

$$\begin{aligned} \sigma_{ab} &= ie^2 \lim_{\omega \rightarrow 0} \lim_{\mathbf{q} \rightarrow 0} \frac{1}{i\omega} (\chi_{J_a J_b} + D_{ab}) \\ &= ie^2 \lim_{\omega \rightarrow 0} \lim_{\mathbf{q} \rightarrow 0} \frac{1}{i\omega} \left\{ \text{Tr}(J_a^q \odot \Delta \odot J_b^q) + \text{Tr}(J_a^q \odot \Delta \odot \Gamma \odot \Delta \odot J_b^q) \right\}, \end{aligned} \quad (2.25)$$

thus involving the ω -limit, $\mathbf{q} \rightarrow 0$ first and then $\omega \rightarrow 0$.

It is worth noticing that in (2.24) the kernel R has been replaced by $\Delta = R - R^q$. In other words, we have been obliged to manipulate RPA in order to build a correspondence with the physical response function and get rid of the unknown bare current vertex and diamagnetic term. From the explicit form (2.8) we find

$$\Delta_{\ell m}(\mathbf{k}; \omega, \mathbf{q}) = \frac{f(\varepsilon_m(\mathbf{k})) - f(\varepsilon_\ell(\mathbf{k} + \mathbf{q}))}{i\omega + (\varepsilon_m(\mathbf{k}) - \varepsilon_\ell(\mathbf{k} + \mathbf{q}))} - \lim_{\mathbf{q} \rightarrow 0} \frac{f(\varepsilon_m(\mathbf{k})) - f(\varepsilon_\ell(\mathbf{k} + \mathbf{q}))}{\varepsilon_m(\mathbf{k}) - \varepsilon_\ell(\mathbf{k} + \mathbf{q})}. \quad (2.26)$$

Since we are interested in small $\mathbf{q}$ and ω , we expand $\varepsilon_\ell(\mathbf{k} + \mathbf{q}) \simeq \varepsilon_\ell(\mathbf{k}) + \mathbf{v}_\ell(\mathbf{k}) \cdot \mathbf{q}$, with $\mathbf{v}_\ell(\mathbf{k}) = \nabla_{\mathbf{k}} \varepsilon_\ell(\mathbf{k})$ the group velocity, so that $f(\varepsilon_\ell(\mathbf{k})) - f(\varepsilon_\ell(\mathbf{k} + \mathbf{q})) \simeq -\frac{\partial f}{\partial \varepsilon_\ell} \mathbf{v}_\ell(\mathbf{k}) \cdot \mathbf{q}$, while the $\mathbf{q} \rightarrow 0$ limit in the second term of (2.26) yields the derivative $\partial f / \partial \varepsilon_\ell$. Hence, for $\ell = m$ and at leading order,

$$\begin{aligned} \Delta_{\ell\ell}(\mathbf{k}; \omega, \mathbf{q}) &\simeq -\frac{\partial f(\varepsilon_\ell(\mathbf{k}))}{\partial \varepsilon_\ell(\mathbf{k})} \frac{\mathbf{v}_\ell(\mathbf{k}) \cdot \mathbf{q}}{i\omega - \mathbf{v}_\ell(\mathbf{k}) \cdot \mathbf{q}} - \frac{\partial f(\varepsilon_\ell(\mathbf{k}))}{\partial \varepsilon_\ell(\mathbf{k})} \\ &= -\frac{\partial f(\varepsilon_\ell(\mathbf{k}))}{\partial \varepsilon_\ell(\mathbf{k})} \frac{i\omega}{i\omega - \mathbf{v}_\ell(\mathbf{k}) \cdot \mathbf{q}}, \end{aligned} \quad (2.27)$$

which is the standard single-band result [67, 68]. On the contrary, for $\ell \neq m$ and assuming $\varepsilon_\ell(\mathbf{k}) \neq \varepsilon_m(\mathbf{k})$ the denominators stay finite as $\mathbf{q} \rightarrow 0$, so we may set $\mathbf{q} = 0$ directly and obtain

$$\begin{aligned} \Delta_{\ell m}(\mathbf{k}; \omega, \mathbf{q}) &\simeq [f(\varepsilon_m(\mathbf{k})) - f(\varepsilon_\ell(\mathbf{k}))] \left(\frac{1}{i\omega + \varepsilon_m(\mathbf{k}) - \varepsilon_\ell(\mathbf{k})} - \frac{1}{\varepsilon_m(\mathbf{k}) - \varepsilon_\ell(\mathbf{k})} \right) \\ &= -i\omega \frac{f(\varepsilon_m(\mathbf{k})) - f(\varepsilon_\ell(\mathbf{k}))}{(i\omega + \varepsilon_m(\mathbf{k}) - \varepsilon_\ell(\mathbf{k}))(\varepsilon_m(\mathbf{k}) - \varepsilon_\ell(\mathbf{k}))} \\ &\simeq -i\omega \frac{f(\varepsilon_m(\mathbf{k})) - f(\varepsilon_\ell(\mathbf{k}))}{(\varepsilon_\ell(\mathbf{k}) - \varepsilon_m(\mathbf{k}))^2}, \end{aligned} \quad (2.28)$$

¹A static, uniform vector potential is a pure gauge and drives no current, so the full response kernel $\chi_{JJ} + D$ must vanish in the q -limit; since D is a constant, this fixes it to $D = -\chi^q$.

which vanishes linearly in ω . Since the ω -limit appears in the conductivity,

$$\begin{aligned}\Delta_{\ell m}^{\omega}(\mathbf{k}) &= \lim_{\omega \rightarrow 0} \lim_{\mathbf{q} \rightarrow 0} \Delta_{\ell m}(\mathbf{k}; \omega, \mathbf{q}) = -\delta_{m\ell} \frac{\partial f(\varepsilon_{\ell}(\mathbf{k}))}{\partial \varepsilon_{\ell}(\mathbf{k})}, \\ \dot{\Delta}_{\ell m}^{\omega}(\mathbf{k}) &= \lim_{\omega \rightarrow 0} \lim_{\mathbf{q} \rightarrow 0} \frac{\partial \Delta_{\ell m}(\mathbf{k}; \omega, \mathbf{q})}{\partial i\omega} = -(1 - \delta_{m\ell}) \frac{f(\varepsilon_m(\mathbf{k})) - f(\varepsilon_{\ell}(\mathbf{k}))}{(\varepsilon_{\ell}(\mathbf{k}) - \varepsilon_m(\mathbf{k}))^2}.\end{aligned}\tag{2.29}$$

In other words, the matrix Δ^{ω} is diagonal, whereas its derivative $\dot{\Delta}^{\omega}$ with respect to ω , evaluated at $\omega = 0$, is off-diagonal. This result is key in the calculation of the Hall conductivity.

Let us first, however, compute the longitudinal conductivity, i.e. the variation of the electric current along the direction, say x , of a uniform static electric field, divided by the field strength. From (2.25), moving to the real-frequency axis $i\omega \rightarrow \omega + i0^+$ with small ω and setting $\mathbf{q} = 0$,

$$\begin{aligned}\sigma_{xx}(\omega) &= i \frac{e^2}{\omega + i0^+} \left\{ \text{Tr}(J_x^q \odot \Delta^{\omega} \odot J_x^q) + \text{Tr}(J_x^q \odot \Delta^{\omega} \odot \Gamma^{\omega} \odot \Delta^{\omega} \odot J_x^q) \right\} \\ &= i \frac{e^2}{\omega + i0^+} \text{Tr}(J_x^q \odot \Delta^{\omega} \odot J_x^{\omega}) \\ &\equiv i \frac{1}{\omega + i0^+} D_{xx},\end{aligned}\tag{2.30}$$

where D_{xx} is the Drude weight and J^{ω} the ω -limit of the current vertex which, through (2.22), satisfies

$$J^{\omega} = J^q + J^q \odot \Delta^{\omega} \odot \Gamma^{\omega} = J^q + \Gamma^{\omega} \odot \Delta^{\omega} \odot J^q.\tag{2.31}$$

We now turn to the Hall conductivity. Adapting the results of Ref. [47], the anti-symmetric combination $(\sigma_{ab} - \sigma_{ba})/2$ defines the element σ_{ab}^H of the anomalous Hall conductivity, which can be shown to be

$$\sigma_{ab}^H = ie^2 \lim_{\omega \rightarrow 0} \lim_{\mathbf{q} \rightarrow 0} \frac{\partial}{\partial i\omega} \left\{ \text{Tr}(J_a^q \odot \Delta \odot J_b^q) + \text{Tr}(J_a^q \odot \Delta \odot \Gamma \odot \Delta \odot J_b^q) \right\}.\tag{2.32}$$

Therefore,

$$\begin{aligned}\sigma_{ab}^H &= ie^2 \left\{ \text{Tr}(J_a^q \odot \dot{\Delta}^{\omega} \odot J_b^q) + \text{Tr}(J_a^q \odot \dot{\Delta}^{\omega} \odot \Gamma^{\omega} \odot \Delta^{\omega} \odot J_b^q) \right. \\ &\quad \left. + \text{Tr}(J_a^q \odot \Delta^{\omega} \odot \Gamma^{\omega} \odot \dot{\Delta}^{\omega} \odot J_b^q) + \text{Tr}(J_a^q \odot \Delta^{\omega} \odot \dot{\Gamma}^{\omega} \odot \Delta^{\omega} \odot J_b^q) \right\},\end{aligned}\tag{2.33}$$

which involves Δ^{ω} and $\dot{\Delta}^{\omega}$ of (2.29). The ω -limit of the derivative of (2.9) is

$$\begin{aligned}\dot{\Gamma}^{\omega} &= f \odot \dot{\Delta}^{\omega} \odot \Gamma^{\omega} + f \odot R^{\omega} \odot \dot{\Gamma}^{\omega} \\ &= \Gamma^{\omega} \odot \dot{\Delta}^{\omega} \odot \Gamma^{\omega}\end{aligned}\tag{2.34}$$

and, substituted into (2.33), gives the compact expression

$$\sigma_{ab}^H = ie^2 \text{Tr}(J_a^{\omega} \odot \dot{\Delta}^{\omega} \odot J_b^{\omega}),\tag{2.35}$$

which again involves the ω -limit of the current vertex (2.31).

Let us finally consider the charge density-density response function. Repeating the above manipulations step by step, but now using the ω -limit of the vertex, one obtains

$$\chi_{\rho\rho} = \chi_{\rho\rho}^\omega + \text{Tr}(\rho^\omega \odot (R - R^\omega) \odot \rho^\omega) + \text{Tr}(\rho^\omega \odot (R - R^\omega) \odot \Gamma \odot (R - R^\omega) \odot \rho^\omega), \quad (2.36)$$

where ρ^ω is the ω -limit of the charge density vertex, ρ_0 the bare one, and

$$\chi_{\rho\rho}^\omega = \text{Tr}(\rho^\omega \odot R^\omega \odot \rho_0) \quad (2.37)$$

the ω -limit of the response function. Charge conservation implies $\chi_{\rho\rho}^\omega = 0$, while the Ward-Takahashi identities fix ρ^ω to the identity matrix in orbital space [67, 68]. Since $R^q - R^\omega = -\Delta^\omega$, see (2.29), the charge compressibility is readily obtained as

$$\begin{aligned} \kappa &= -\chi_{\rho\rho}^q = \text{Tr}(\Delta^\omega) - \text{Tr}(\Delta^\omega \odot \Gamma^q \odot \Delta^\omega) \\ &= -\frac{1}{V} \sum_{\mathbf{k}\ell} \frac{\partial f(\varepsilon_\ell(\mathbf{k}))}{\partial \varepsilon_\ell(\mathbf{k})} - \frac{1}{V^2} \sum_{\mathbf{k}\mathbf{k}'\ell\ell'} \frac{\partial f(\varepsilon_\ell(\mathbf{k}))}{\partial \varepsilon_\ell(\mathbf{k})} \Gamma_{\ell\ell',\ell'\ell}^q(\mathbf{k}, \mathbf{k}') \frac{\partial f(\varepsilon_{\ell'}(\mathbf{k}'))}{\partial \varepsilon_{\ell'}(\mathbf{k}')}, \end{aligned} \quad (2.38)$$

which is the conventional result of Fermi-liquid theory: the compressibility is not merely the quasiparticle density of states at the chemical potential, but acquires a correction from the quasiparticle interaction.

Equations (2.30), (2.35) and (2.38) are the central results of this construction: every physical transport and thermodynamic coefficient is expressed through the q - and ω -limits of the current and density vertices, the only objects for which the HF+RPA description can be rigorously identified with the physical Fermi liquid. In particular, the anomalous Hall conductivity (2.35) is governed by the ω -limit J^ω of the current vertex, a point whose physical content we unfold in the next subsection.

2.1.2 Anomalous Hall conductivity of a multiband Fermi liquid

We have seen that, by means of the Ward-Takahashi identities, the q -limit of the fully interacting physical current vertex, multiplied by the quasiparticle residue and hereafter denoted $\hat{J}^q(\mathbf{k})$, corresponds to $\nabla_{\mathbf{k}} \hat{H}_*(\mathbf{k})$ for the quasiparticles [67, 68]. In the diagonal HF basis defined by (2.6) that correspondence reads

$$\begin{aligned} \hat{J}^q(\mathbf{k}) &\equiv \hat{U}(\mathbf{k})^\dagger \nabla_{\mathbf{k}} \hat{H}_*(\mathbf{k}) \hat{U}(\mathbf{k}) \\ &= \hat{U}(\mathbf{k})^\dagger \nabla_{\mathbf{k}} (\hat{U}(\mathbf{k}) \hat{\varepsilon}_*(\mathbf{k}) \hat{U}(\mathbf{k})^\dagger) \hat{U}(\mathbf{k}) \\ &= \nabla_{\mathbf{k}} \hat{\varepsilon}_*(\mathbf{k}) - [\hat{\varepsilon}_*(\mathbf{k}), \hat{U}(\mathbf{k})^\dagger \nabla_{\mathbf{k}} \hat{U}(\mathbf{k})] \\ &\equiv \nabla_{\mathbf{k}} \hat{\varepsilon}_*(\mathbf{k}) + i [\hat{\varepsilon}_*(\mathbf{k}), \hat{\mathcal{A}}^0(\mathbf{k})], \end{aligned} \quad (2.39)$$

where the first term is diagonal and the second off-diagonal in the band indices. Here, the hermitian operator $\hat{\mathcal{A}}^0(\mathbf{k}) = i \hat{U}(\mathbf{k})^\dagger \nabla_{\mathbf{k}} \hat{U}(\mathbf{k})$ is the bare Berry connection of the quasiparticles, whose matrix elements are also equal to

$$\mathcal{A}_{\ell m}^0(\mathbf{k}) = i \langle \psi_\ell(\mathbf{k}) | \nabla_{\mathbf{k}} \psi_m(\mathbf{k}) \rangle = -i \langle \nabla_{\mathbf{k}} \psi_\ell(\mathbf{k}) | \psi_m(\mathbf{k}) \rangle, \quad (2.40)$$

through which the diagonal part of the bare Berry curvature is $\Omega_{\ell\ell}^0(\mathbf{k}) = -\nabla_{\mathbf{k}} \times \mathcal{A}_{\ell\ell}^0(\mathbf{k})$. The reason why we have reformulated Landau's Fermi liquid theory in such a more complex language is to make it clear that the quasiparticles are interacting, even though the interaction is treated within HF plus RPA. This point becomes important when one wants to compute topological observables. As already mentioned, the first temptation is to use the eigenstates $|\psi_{\ell}(\mathbf{k})\rangle$ and calculate the topological invariants as one would do for non-interacting electrons, see (2.40). However, this procedure might be incorrect just because the quasiparticles do interact with each other.

A more rigorous approach is to directly calculate the anomalous Hall conductivity as dictated by Landau's Fermi-liquid theory. Specialising the master formula (2.35) to the off-diagonal form of $\dot{\Delta}^{\omega}$ in (2.29), the matrix elements $\sigma_{ab}^H = -\sigma_{ba}^H$, with $a \neq b$ labelling the spatial components of the Hall conductivity tensor, read explicitly

$$\begin{aligned}\sigma_{ab}^H &= -i \frac{e^2}{V} \sum_{\mathbf{k}} \sum_{\ell \neq m} J_{a\ell m}^{\omega}(\mathbf{k}) \frac{f(\varepsilon_{\ell}(\mathbf{k})) - f(\varepsilon_m(\mathbf{k}))}{(\varepsilon_m(\mathbf{k}) - \varepsilon_{\ell}(\mathbf{k}))^2} J_{bml}^{\omega}(\mathbf{k}) \\ &= -i \frac{e^2}{V} \sum_{\mathbf{k}} \sum_{\ell \neq m} f(\varepsilon_{\ell}(\mathbf{k})) \frac{J_{a\ell m}^{\omega}(\mathbf{k}) J_{bml}^{\omega}(\mathbf{k}) - J_{b\ell m}^{\omega}(\mathbf{k}) J_{aml}^{\omega}(\mathbf{k})}{(\varepsilon_m(\mathbf{k}) - \varepsilon_{\ell}(\mathbf{k}))^2} \\ &\equiv \frac{e^2}{V} \sum_{\mathbf{k}\ell} f(\varepsilon_{\ell}(\mathbf{k})) \epsilon_{abc} \Omega_{c\ell\ell}(\mathbf{k}),\end{aligned}\tag{2.41}$$

where $f(x)$ is the Fermi distribution function and

$$\Omega_{\ell\ell}(\mathbf{k}) = -i \sum_{m \neq \ell} \frac{J_{\ell m}^{\omega}(\mathbf{k}) \times J_{m\ell}^{\omega}(\mathbf{k})}{(\varepsilon_m(\mathbf{k}) - \varepsilon_{\ell}(\mathbf{k}))^2}\tag{2.42}$$

is therefore the true quasiparticle Berry curvature. The dynamic, ω -limit of the current vertex, the opposite of the q -limit, is related to (2.39) through (2.31), specifically

$$J_{\ell m}^{\omega}(\mathbf{k}) = J_{\ell m}^q(\mathbf{k}) - \frac{1}{V} \sum_{\mathbf{k}'n} \Gamma_{\ell n, nm}^{\omega}(\mathbf{k}', \mathbf{k}) \nabla_{\mathbf{k}'} f(\varepsilon_n(\mathbf{k}')), \tag{2.43}$$

where Γ^{ω} is the ω -limit of the reducible scattering vertex (2.7). The term in (2.42) with the bare current vertices, i.e. $\Gamma^{\omega} = 0$ in (2.43), reproduces the bare Berry curvature $\Omega_{\ell\ell}^0(\mathbf{k})$, while the additional terms correspond to the desired Fermi-liquid corrections and indeed derive, as the second term in (2.43) makes evident, from the quasiparticle Fermi surface. It is therefore reasonable to argue that also the corrections to the anomalous Hall conductivity come from the quasiparticle Fermi surface, though this conclusion seems not immediately obvious looking at (2.41) and (2.43). Indeed, it may seem counterintuitive that a quantity evaluated within Landau's theory of Fermi liquids could have contributions from bands that do not cross the chemical potential. However, we believe such a paradox to be merely apparent, and in the next section we analyse a specific example that explicitly confirms this surmise.

Nonetheless, we emphasise that, while the corrections do derive from the quasiparticles at the Fermi surface, equation (2.41) accounts also for cases where there are occupied

bands that contribute to the anomalous Hall conductivity. It might at first look odd that the contribution of an occupied band may not be quantised because of its interaction with the bands crossing the chemical potential, but this does not contradict any physical principle as long as the contribution becomes again quantised when no band crosses the chemical potential any more, which is clearly the case here, see (2.43).

2.2 An explicit toy model calculation

We now specialise the general discussion to a concrete example, the Bernevig-Hughes-Zhang (BHZ) model [31] of a quantum spin-Hall insulator on a square lattice introduced in Chapter 1. Here we assume the model with full spin polarisation, so that only the spin-up bands are occupied, and at density $n = 1 + \delta$, in which case it describes a topological metal with broken time-reversal symmetry. The Hamiltonian for the spin-up quasiparticles is taken to be

$$\begin{aligned}\hat{H}_*(\mathbf{k}) &= (\varepsilon(\mathbf{k}) - \mu)\sigma_0 + (M - t(\mathbf{k}))\sigma_3 + \lambda(\mathbf{k})\sin k_x\sigma_1 - \lambda(\mathbf{k})\sin k_y\sigma_2 \\ &= (\varepsilon(\mathbf{k}) - \mu)\sigma_0 + \mathbf{B}(\mathbf{k}) \cdot \boldsymbol{\sigma},\end{aligned}\tag{2.44}$$

where μ crosses either the valence or the conduction band, σ_0 is the identity and σ_a ($a = 1, 2, 3$) the Pauli matrices acting on the orbital space, and

$$\begin{aligned}\mathbf{B}(\mathbf{k}) &= (\lambda(\mathbf{k})\sin k_x, -\lambda(\mathbf{k})\sin k_y, M - t(\mathbf{k})) \\ &= B(\mathbf{k})(\cos \phi(\mathbf{k})\sin \theta(\mathbf{k}), \sin \phi(\mathbf{k})\sin \theta(\mathbf{k}), \cos \theta(\mathbf{k})) \\ &= B(\mathbf{k})(\sin \theta(\mathbf{k})\mathbf{v}_2(\mathbf{k}) + \cos \theta(\mathbf{k})\mathbf{v}_3(\mathbf{k})).\end{aligned}\tag{2.45}$$

Here $\mathbf{v}_2(\mathbf{k}) = (\cos \phi(\mathbf{k}), \sin \phi(\mathbf{k}), 0)$ and $\mathbf{v}_3(\mathbf{k}) = (0, 0, 1)$ are orthogonal unit vectors that, together with $\mathbf{v}_1(\mathbf{k}) = \mathbf{v}_2(\mathbf{k}) \times \mathbf{v}_3(\mathbf{k})$, form a basis; correspondingly σ_0 and $\mathbf{v}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}$, $a = 1, 2, 3$, form a basis of 2×2 matrices, and to lighten the notation we set $\mathbf{v}_0(\mathbf{k}) \cdot \boldsymbol{\sigma} \equiv \sigma_0$.

The Hamiltonian (2.44) is assumed to be invariant under inversion $\mathcal{I}$, $\mathbf{k} \rightarrow -\mathbf{k}$ and $\sigma_a \rightarrow -\sigma_a$ for $a = 1, 2$, and under fourfold rotations $\mathcal{C}_4$, $k_x \rightarrow k_y \wedge k_y \rightarrow -k_x$ and $\sigma_1 \rightarrow -\sigma_2 \wedge \sigma_2 \rightarrow \sigma_1$. This requires the parameters $\varepsilon(\mathbf{k})$, $t(\mathbf{k})$ and $\lambda(\mathbf{k})$ to be invariant under both $\mathcal{I}$ and $\mathcal{C}_4$. In addition, in order to clearly distinguish μ and M from $\varepsilon(\mathbf{k})$ and $t(\mathbf{k})$, respectively, we assume the latter to average to zero over the Brillouin zone. The Hamiltonian is diagonalised by the unitary transformation

$$\hat{U}(\mathbf{k}) = e^{i\frac{\theta(\mathbf{k})}{2}\mathbf{v}_1(\mathbf{k}) \cdot \boldsymbol{\sigma}} = \cos \frac{\theta(\mathbf{k})}{2} + i \sin \frac{\theta(\mathbf{k})}{2} \mathbf{v}_1(\mathbf{k}) \cdot \boldsymbol{\sigma},\tag{2.46}$$

namely $\hat{U}(\mathbf{k})^\dagger \hat{H}_*(\mathbf{k}) \hat{U}(\mathbf{k}) = (\varepsilon(\mathbf{k}) - \mu)\sigma_0 + B(\mathbf{k})\sigma_3$. We readily find that

$$\begin{aligned}\hat{\mathcal{A}}^0(\mathbf{k}) &= i\hat{U}(\mathbf{k})^\dagger \nabla_{\mathbf{k}} \hat{U}(\mathbf{k}) = -\frac{\nabla_{\mathbf{k}} \theta(\mathbf{k})}{2} \mathbf{v}_1(\mathbf{k}) \cdot \boldsymbol{\sigma} \\ &\quad - \frac{\nabla_{\mathbf{k}} \phi(\mathbf{k})}{2} \sin \theta(\mathbf{k}) \mathbf{v}_2(\mathbf{k}) \cdot \boldsymbol{\sigma} - \nabla_{\mathbf{k}} \phi(\mathbf{k}) \sin^2 \frac{\theta(\mathbf{k})}{2} \mathbf{v}_3(\mathbf{k}) \cdot \boldsymbol{\sigma} \\ &= \sum_{a=1}^3 \mathcal{A}_a^0(\mathbf{k}) \mathbf{v}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}.\end{aligned}\tag{2.47}$$

We can make a similar expansion for the current vertices,

$$\hat{J}^q(\mathbf{k}) = \sum_{a=0}^3 J_a^q(\mathbf{k}) \mathbf{v}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad \hat{J}^\omega(\mathbf{k}) = \sum_{a=0}^3 J_a^\omega(\mathbf{k}) \mathbf{v}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (2.48)$$

where $J_0^q(\mathbf{k}) = \nabla_{\mathbf{k}} \varepsilon(\mathbf{k})$, $J_3^q(\mathbf{k}) = \nabla_{\mathbf{k}} B(\mathbf{k})$ and $J_a^q(\mathbf{k}) = 2B(\mathbf{k}) \epsilon_{ab3} \mathcal{A}_b^0(\mathbf{k})$ for $a = 1, 2$. In the top panel of Fig. 2.1 we show the band structure of (2.44) at $\varepsilon(\mathbf{k}) = 0$, $M = 1$, $t(\mathbf{k}) = \cos k_x + \cos k_y$ and $\lambda(\mathbf{k}) = 0.2$, indicating the chemical potential μ for the different hole-doping levels and the corresponding Fermi surfaces. In the bottom panel we draw the momentum distribution of the bare Berry curvature of the valence band, as well as its integral, in units of 2π , over the occupied Fermi volume as a function of $\mu < 0$.

We note that $\mathbf{v}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}$, $a = 0, \dots, 3$, are invariant under both $\mathcal{I}$ and $\mathcal{C}_4$, while $\nabla_{\mathbf{k}} \phi(\mathbf{k})$ and $\nabla_{\mathbf{k}} \theta(\mathbf{k})$ transform as conventional vectors. Since the f -parameters contribute to the quasiparticle Hamiltonian (2.44) through the mean-field decoupling, the form of $\mathbf{B}(\mathbf{k})$ in (2.45) implies that the most general $\hat{f}$ -tensor in the original basis must be of the form

$$\hat{f}(\mathbf{k}, \mathbf{k}') = \sum_{a,b=0,2,3} f_{ab}(\mathbf{k}, \mathbf{k}') (\mathbf{v}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}) \otimes (\mathbf{v}_b(\mathbf{k}') \cdot \boldsymbol{\sigma}), \quad (2.49)$$

thus lacking terms that involve $\mathbf{v}_1(\mathbf{k}) \cdot \boldsymbol{\sigma}$, and where symmetry only requires that the expansion coefficients be invariant under $\mathcal{I}$ and $\mathcal{C}_4$. Upon rotation to the HF basis, (2.49) keeps the same form with modified coefficients, which we still denote $f_{ab}(\mathbf{k}, \mathbf{k}')$ for simplicity. We can further identify two distinct tensors, $\hat{f}^0(\mathbf{k}, \mathbf{k}') = \hat{f}^0(-\mathbf{k}, \mathbf{k}') = \hat{f}^0(\mathbf{k}, -\mathbf{k}')$ and $\hat{f}^1(\mathbf{k}, \mathbf{k}') = -\hat{f}^1(-\mathbf{k}, \mathbf{k}') = -\hat{f}^1(\mathbf{k}, -\mathbf{k}')$, using the same notation as in conventional single-band Fermi liquids [85]. It is precisely $\hat{f}^1$ that may contribute to (2.43), which, without loss of generality, can be taken in the HF basis of the form

$$\hat{f}^1(\mathbf{k}, \mathbf{k}') = \sum_{a,b=0,2,3} f_{ab}^1(\mathbf{k}, \mathbf{k}') J_a^q(\mathbf{k}) \cdot J_b^q(\mathbf{k}') (\mathbf{v}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}) \otimes (\mathbf{v}_b(\mathbf{k}') \cdot \boldsymbol{\sigma}), \quad (2.50)$$

where, for consistency, $f_{ab}^1(\mathbf{k}, \mathbf{k}') = f_{ab}^1(-\mathbf{k}, \mathbf{k}') = f_{ab}^1(\mathbf{k}, -\mathbf{k}')$ vary in momentum space orthogonally to the corresponding currents, i.e.

$$J_a^q(\mathbf{k}) \cdot \nabla_{\mathbf{k}} f_{ab}^1(\mathbf{k}, \mathbf{k}') = \nabla_{\mathbf{k}'} f_{ab}^1(\mathbf{k}, \mathbf{k}') \cdot J_b^q(\mathbf{k}') = 0, \quad (2.51)$$

for $a, b = 0, 2, 3$. In reality, only the components f_{ab}^1 with $a = 0, 2, 3$ and $b = 0, 3$ contribute to (2.43), in which case (2.7) implies $\Gamma_{ab}^{1\omega}(\mathbf{k}, \mathbf{k}') \equiv f_{ab}^1(\mathbf{k}, \mathbf{k}')$. It is worth remarking that $\hat{f}(\mathbf{k}, \mathbf{k}')$ in (2.49) contributes to $\hat{H}_*(\mathbf{k})$ in (2.44) through the HF self-energy, see (2.5). Therefore, if we reasonably assume that the HF ground state carries no current, the mean-field terms generated by $\hat{f}^1(\mathbf{k}, \mathbf{k}')$ must vanish at self-consistency, which requires, at the very least, non-singular coefficients $f_{ab}^1(\mathbf{k}, \mathbf{k}')$. This observation will be useful later on.

We further define the diagonal matrix $\hat{P}(\mathbf{k})$ with elements $f(\varepsilon_\ell(\mathbf{k}))$, which we can write as

$$\begin{aligned} \hat{P}(\mathbf{k}) &= \frac{f(\varepsilon_1(\mathbf{k})) + f(\varepsilon_2(\mathbf{k}))}{2} \mathbf{v}_0(\mathbf{k}) \cdot \boldsymbol{\sigma} + \frac{f(\varepsilon_1(\mathbf{k})) - f(\varepsilon_2(\mathbf{k}))}{2} \mathbf{v}_3(\mathbf{k}) \cdot \boldsymbol{\sigma} \\ &\equiv P_0(\mathbf{k}) \mathbf{v}_0(\mathbf{k}) \cdot \boldsymbol{\sigma} + P_3(\mathbf{k}) \mathbf{v}_3(\mathbf{k}) \cdot \boldsymbol{\sigma}, \end{aligned} \quad (2.52)$$

where the conduction band 1 corresponds to $\sigma_3 = +1$ with energy $\varepsilon_1(\mathbf{k}) = \varepsilon(\mathbf{k}) - \mu + B(\mathbf{k})$, and the valence band 2 to $\sigma_3 = -1$ with $\varepsilon_2(\mathbf{k}) = \varepsilon(\mathbf{k}) - \mu - B(\mathbf{k})$. With these definitions, (2.43) transforms into an equation for each component in the matrix basis, specifically, and exploiting the spatial symmetries,

$$\begin{aligned} J_a^\omega(\mathbf{k}) &= J_a^q(\mathbf{k}) - (1 - \delta_{a,1}) \frac{2}{V} \sum_{\mathbf{k}'} \sum_{b=0,3} f_{ab}^1(\mathbf{k}, \mathbf{k}') \nabla_{\mathbf{k}'} P_b(\mathbf{k}') (J_a^q(\mathbf{k}) \cdot J_b^q(\mathbf{k}')) \\ &= J_a^q(\mathbf{k}) \left[1 - (1 - \delta_{a,1}) \frac{1}{V} \sum_{\mathbf{k}'} \sum_{b=0,3} f_{ab}^1(\mathbf{k}, \mathbf{k}') \nabla_{\mathbf{k}'} P_b(\mathbf{k}') \cdot J_b^q(\mathbf{k}') \right] \\ &\equiv J_a^q(\mathbf{k}) \left[1 + (1 - \delta_{a,1}) \frac{F_a^1(\mathbf{k})}{2} \right]. \end{aligned} \quad (2.53)$$

The anomalous Hall conductivity $\sigma^H = \sigma_{xy}^H$ in (2.41) can then be written as

$$\begin{aligned} \sigma^H &= -i \frac{e^2}{V} \sum_{\mathbf{k}} \sum_{a,b=1}^2 \frac{J_{xa}^\omega(\mathbf{k}) J_{yb}^\omega(\mathbf{k})}{4B(\mathbf{k})^2} \text{Tr} \left([P_3(\mathbf{k}) \mathbf{v}_3 \cdot \boldsymbol{\sigma}, \mathbf{v}_a \cdot \boldsymbol{\sigma}] \mathbf{v}_b \cdot \boldsymbol{\sigma} \right) \\ &= \frac{e^2}{2V} \sum_{\mathbf{k}} \sum_{a,b=1}^2 \frac{P_3(\mathbf{k})}{B(\mathbf{k})^2} \epsilon_{ab3} J_a^\omega(\mathbf{k}) \times J_b^\omega(\mathbf{k}) \cdot \mathbf{v}_3 \\ &= -\frac{e^2}{V} \sum_{\mathbf{k}} P_3(\mathbf{k}) \left(1 + \frac{F_2^1(\mathbf{k})}{2} \right) \nabla_{\mathbf{k}} \times (\cos \theta(\mathbf{k}) \nabla_{\mathbf{k}} \phi(\mathbf{k})) \cdot \mathbf{v}_3 \\ &= \frac{e^2}{V} \sum_{\mathbf{k}} \cos \theta(\mathbf{k}) \left(1 + \frac{F_2^1(\mathbf{k})}{2} \right) \nabla_{\mathbf{k}} P_3(\mathbf{k}) \times \nabla_{\mathbf{k}} \phi(\mathbf{k}) \cdot \mathbf{v}_3 \\ &\quad + \frac{e^2}{2V} \sum_{\mathbf{k}} \cos \theta(\mathbf{k}) P_3(\mathbf{k}) \nabla_{\mathbf{k}} F_2^1(\mathbf{k}) \times \nabla_{\mathbf{k}} \phi(\mathbf{k}) \cdot \mathbf{v}_3. \end{aligned} \quad (2.54)$$

The first term in the last equality of (2.54) is a genuine Fermi-surface contribution as it contains $\nabla_{\mathbf{k}} P_3(\mathbf{k})$. Concerning the last term, we recall that $J_2^q(\mathbf{k}) \propto \mathcal{A}_1^0(\mathbf{k}) \propto \nabla_{\mathbf{k}} \theta(\mathbf{k})$, so that the orthogonality condition (2.51) forces $\nabla_{\mathbf{k}} F_2^1(\mathbf{k})$ to be perpendicular to $\nabla_{\mathbf{k}} \theta(\mathbf{k})$. In two dimensions this implies $\nabla_{\mathbf{k}} F_2^1(\mathbf{k}) \times \nabla_{\mathbf{k}} \phi(\mathbf{k}) \propto \nabla_{\mathbf{k}} \theta(\mathbf{k}) \cdot \nabla_{\mathbf{k}} \phi(\mathbf{k})$, which is odd under the mirror exchange $k_x \leftrightarrow k_y$. It therefore averages to zero upon summing over $\mathbf{k}$, since $P_3(\mathbf{k})$ and $\cos \theta(\mathbf{k})$ are both invariant under the same exchange. In conclusion,

$$\sigma^H = \frac{e^2}{V} \sum_{\mathbf{k}} \left(1 + \frac{F_2^1(\mathbf{k})}{2} \right) \cos \theta(\mathbf{k}) \nabla_{\mathbf{k}} P_3(\mathbf{k}) \times \nabla_{\mathbf{k}} \phi(\mathbf{k}) \cdot \mathbf{v}_3 \equiv \sigma_0^H \left(1 + \frac{F_2^1}{2} \right), \quad (2.55)$$

where σ_0^H is the bare value, i.e. neglecting the vertex corrections, and F_2^1 is a weighted average over the Fermi surfaces. Therefore, in the model (2.44) we can explicitly verify that the corrections to the anomalous Hall conductivity only derive from the quasiparticle Fermi surface, as we earlier conjectured. We believe that this result has a more general validity.

For completeness, the Drude weight $D_{xx} = D_{yy} = D$ can be readily found through

(2.30),

$$D = D_0 \left(1 + \frac{F^1}{2} \right), \quad (2.56)$$

where

$$D_0 = -\frac{e^2}{2V} \sum_{\mathbf{k}} \sum_{\ell=1}^2 \frac{\partial f(\varepsilon_{\ell}(\mathbf{k}))}{\partial \varepsilon_{\ell}(\mathbf{k})} \nabla_{\mathbf{k}\varepsilon_{\ell}(\mathbf{k})} \cdot \nabla_{\mathbf{k}\varepsilon_{\ell}(\mathbf{k})} = \frac{e^2}{2V} \sum_{\mathbf{k}} \sum_{\ell=1}^2 f(\varepsilon_{\ell}(\mathbf{k})) \nabla_{\mathbf{k}\varepsilon_{\ell}(\mathbf{k})}^2 \quad (2.57)$$

is the bare value, and F^1 is again a weighted average over the Fermi surfaces of $F_0^1(\mathbf{k})$ and $F_3^1(\mathbf{k})$, see (2.53). In this case, $F^1/2$ is the correction to the optical mass with respect to the quasiparticle effective one, defined through the last equality in (2.57).

We emphasise that the Fermi-liquid corrections to both the anomalous Hall conductivity (2.55) and the Drude weight (2.56) stem from the fact that we are studying the response to a uniform electric field, which has to be evaluated in the ω -limit. As a consequence, the dressed current vertex that enters the response functions is J^{ω} instead of J^q , the latter being the one fixed by the Ward-Takahashi identity. In a Fermi liquid $J^{\omega} \neq J^q$ because the quasiparticle Fermi surface induces a non-analyticity at $\omega = \mathbf{q} = 0$, which is the key to the microscopic derivation of Landau's Fermi-liquid theory [67, 68].

To conclude, we mention that, had we considered the same model without explicitly breaking time-reversal symmetry, or models sharing similar topological ingredients, we could still discuss topological properties such as the non-quantised intrinsic component of the spin Hall conductivity [86, 87].

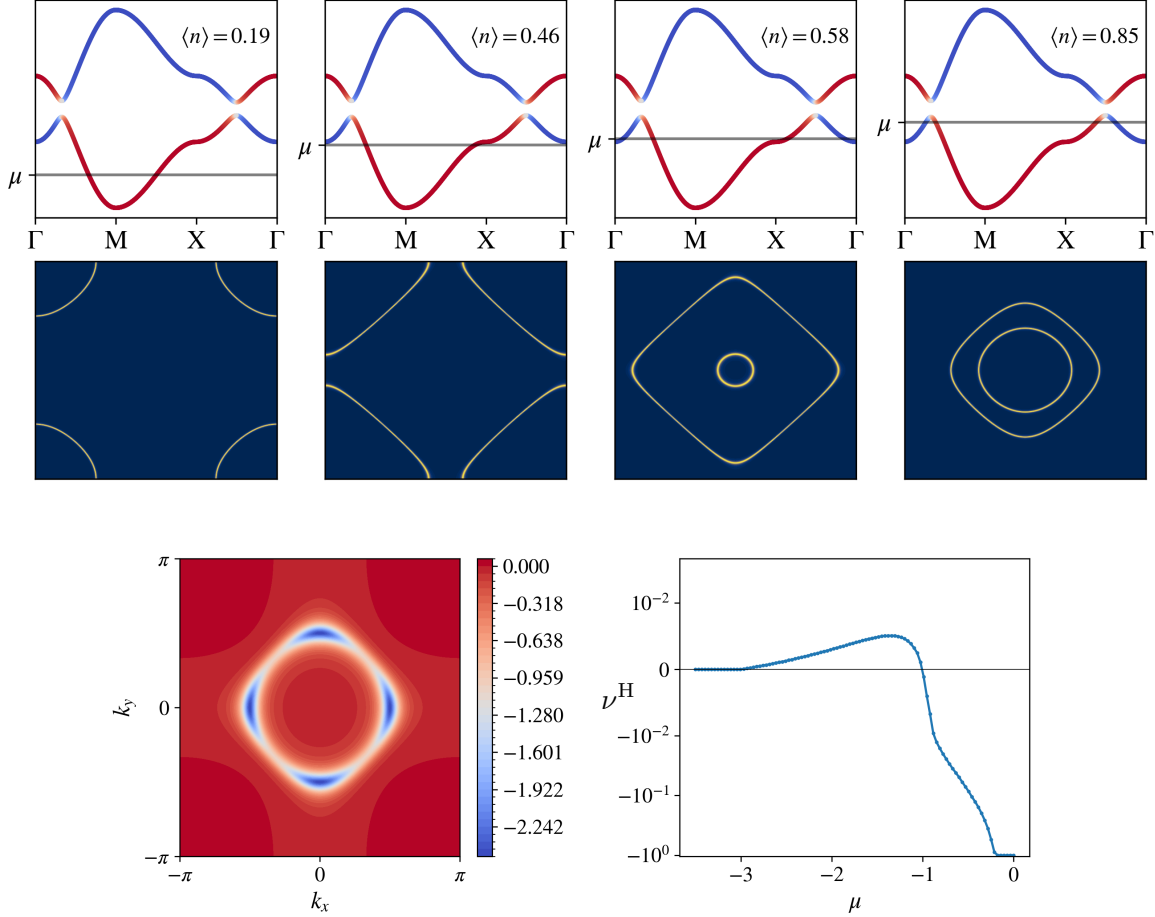


Figure 2.1: Top panel: band structures of (2.44) with $\varepsilon(\mathbf{k}) = 0$, $M = 1$, $t(\mathbf{k}) = \cos k_x + \cos k_y$ and $\lambda(\mathbf{k}) = 0.2$ (top), and Fermi surfaces (bottom) for different values of μ corresponding to hole doping, the average density $\langle n \rangle$ being indicated. Bottom panel: momentum-space distribution of the bare Berry curvature $\Omega^0(\mathbf{k})$ of the valence band (left); integral ν^H of the bare Berry curvature in units of 2π over the occupied Fermi volume (right) as a function of $\mu < 0$. When $2|\mu|$ is smaller than the gap, $\nu^H = -1$ keeps its quantised value, otherwise it deviates, reaching zero when the valence band empties at $\mu = -3$. In reality ν^H crosses zero also when the Fermi surface changes character, from hole-like to electron-like. We also note that $\Omega^0(\mathbf{k})$ of the valence band is peaked in magnitude at the top of the band, where the orbital character changes, which explains the fast decrease in magnitude upon hole doping.

2.3 Conclusions

We have shown that Landau’s theory of Fermi liquids naturally accounts for interaction-induced corrections to the intrinsic anomalous Hall conductivity of topological metals. These corrections arise from the residual interactions among quasiparticles, just as they do for conventional thermodynamic susceptibilities and longitudinal transport coefficients, such as the compressibility and the Drude weight. Consequently, the intrinsic anomalous Hall conductivity cannot be expressed solely in terms of the Berry phases acquired by quasiparticles on the Fermi surface, as one might intuitively expect [35], and the bare Chern number of the occupied bands. Both contributions are renormalised by interactions with the quasiparticles at the chemical potential. This renormalisation reflects the well-known distinction between the static and dynamic limits of linear-response functions in metals.

The corrections uncovered in this chapter constitute the metallic counterpart of recent results for two-dimensional quantum anomalous Hall insulators [47, 83]. In such systems, the Chern number does not necessarily coincide with the topological invariant [45, 46, 63] defined by the winding number $W[G]$ of the map $(\varepsilon, \mathbf{k}) \rightarrow \hat{G}(i\varepsilon, \mathbf{k})$ constructed from the fully interacting Green’s function. As shown in Ref. [47], this winding number is equal to that of the quasiparticle Green’s function $\hat{G}(i\varepsilon, \mathbf{k})$, obtained by filtering out the quasiparticle residue. Upon doping, $W[\hat{G}]$ reduces, in units of $e^2/2\pi$, to the non-quantised bare contribution σ_0^H . Correspondingly, the corrections identified in Refs. [47, 83] reduce to the Fermi-liquid corrections derived here. The present analysis therefore shows how the topological information encoded in the Green’s function survives in the metallic phase: It fixes the bare contribution to the anomalous Hall conductivity, which is subsequently dressed by residual quasiparticle interactions through the f -parameters.

These results also bear directly on the puzzle discussed at the beginning of this chapter. Certain correlated Mott insulators exhibit a vanishing Hall conductance, $\sigma^H = 0$, despite having a finite winding number, $W[G] \neq 0$, carried by in-gap bands of Green’s-function zeros [30, 47, 55]. Applying the formalism developed here to a metal continuously connected to such an insulator as the doping $\delta \rightarrow 0$ could, in principle, reconcile these two properties. Indeed, since

$$\sigma^H = \sigma_0^H \left(1 + \frac{F_2^1}{2} \right), \quad (2.58)$$

while $\sigma_0^H \propto W[\hat{G}_*]$ remains finite, obtaining $\sigma^H \rightarrow 0$ would require the Fermi-liquid correction to approach $F_2^1 \rightarrow -2$.

This is not, however, the only conceivable mechanism. The same behaviour could instead arise from a singularity of the f^1 vertex as the Mott transition is approached, rather than from a regular Fermi-liquid renormalisation. Distinguishing between these scenarios requires a microscopic determination of the f -parameters, which lies beyond the scope of the present work. A detailed investigation of this issue is therefore left for future studies.

CHAPTER 3

Static and dynamical properties of a strong-coupling impurity solver for dynamical mean-field theory

In this chapter, we discuss a deterministic strong-coupling impurity solver for dynamical mean-field theory leveraging a pseudoparticle representation of the local many-body states. The method provides access to the partition function and hence to thermodynamic quantities such as the free energy and the entropy, notoriously difficult to obtain with stochastic Monte Carlo solvers. We assess its accuracy and limitations on the single-band Hubbard model. This chapter is based on Ref. [41].

Introduction

The effective one-body descriptions exploited in the previous chapters ultimately rely on our ability to solve strongly correlated electron models. Dynamical mean-field theory (DMFT) is one of the most successful non-perturbative frameworks for this purpose. It maps a correlated lattice model onto a quantum impurity embedded in a self-consistently determined bath and becomes exact in the limit of infinite lattice coordination [26, 40]. Although this mapping replaces the original lattice problem by a conceptually simpler local one, the resulting impurity problem remains fully interacting and nontrivial. Its solution therefore constitutes the central computational step of any DMFT calculation.

The choice of impurity solver determines not only the numerical accuracy and computational cost of the calculation, but also which physical quantities can be obtained reliably. An ideal solver should combine high accuracy with a manageable computational cost, remain applicable at low temperatures and for general multiorbital Hamiltonians, and provide access to both dynamical observables and thermodynamic potentials.

A broad range of approaches has been introduced since the formulation of DMFT, including exact diagonalization [88, 89], the numerical renormalization group [90, 91], and continuous-time quantum Monte Carlo methods [72, 92, 93]. Among these, continuous-time Monte Carlo has become the standard choice for a large class of DMFT appli-

cations because of its flexibility and its numerically exact treatment of the impurity problem. Its stochastic formulation, however, entails some structural limitations. First, the statistical error sets a floor on the accuracy attainable for the Matsubara-axis self-energy or Green’s function, which in turn amplifies the ill-posedness of their analytic continuation to real frequencies. Second, general multiorbital Hamiltonians or off-diagonal hybridization functions may lead to a fermionic sign problem. Together with the steep increase of the computational cost at large inverse temperature, typically proportional to β^3 , this can make low-temperature calculations prohibitively expensive. These difficulties are especially relevant in systems with substantial spin-orbit coupling, including several proposed topological Mott insulators [94–96].

Another limitation, of particular importance in the present work, concerns thermodynamic potentials. Monte Carlo (MC) algorithms sample configurations according to normalized statistical weights and therefore do not directly determine the absolute value of the partition function. As a result, quantities derived from it, such as the free energy, cannot be obtained from a single calculation. They must instead be reconstructed by thermodynamic integration along a suitable path, for example by combining calculations performed at many different temperatures or interaction strengths. This is a serious practical obstacle, because the free energy is precisely the quantity whose minimization discriminates between competing phases at finite temperature. Direct access to the free energy is therefore essential to locate phase transitions and to resolve the thermodynamic stability of competing phases, such as coexisting metallic and insulating solutions, or competing magnetic and superconducting orders, a situation that is the rule rather than the exception in realistic materials calculations.

These considerations motivate the development of deterministic approaches that complement stochastic impurity solvers. Because they do not rely on Monte Carlo sampling, deterministic methods are free from statistical noise and the sign problem. While generally less flexible than MC methods, which remain numerically exact for arbitrary impurity problems, deterministic solvers can be particularly powerful and even outperform MC in specific regimes.

The chapter is organized as follows. In Sec. 3.1 we set up the strong-coupling expansion of the Anderson impurity problem and introduce the pseudoparticle representation that turns the hybridization into the expansion parameter, with the atomic limit as the unperturbed reference. In Sec. 3.2 we show how physical observables and thermodynamic potentials are extracted within this framework, exploiting the explicit evaluation of the partition function to gain direct access to the impurity and lattice free energies and to the entropy. In Sec. 3.3 we benchmark the solver on the single-band Hubbard model on the Bethe lattice.

3.1 Strong-coupling expansion and pseudoparticle representation

Within DMFT, the lattice self-energy is approximated as momentum independent,

$$\Sigma_{\text{latt}}(\mathbf{k}, i\omega_n) \rightarrow \Sigma_{\text{latt}}(i\omega_n), \quad (3.1)$$

this approximation being exact in the limit of infinite lattice coordination [26, 40]. $i\omega_n = i(2n+1)\pi/\beta$ are the fermionic Matsubara frequencies, with $n \in \mathbb{Z}$ and $\beta = 1/T$ the inverse temperature ($k_B = 1$). For a generic multiorbital system, the corresponding local lattice Green's function is given in Matsubara frequency by

$$\mathbf{G}_{\text{loc}}(i\omega_n) = \frac{1}{N_k} \sum_{\mathbf{k}} [(i\omega_n - \mu) \mathbf{I} - \mathbf{H}_{\mathbf{k}} - \Sigma_{\text{latt}}(i\omega_n)]^{-1}, \quad (3.2)$$

where $\mathbf{H}_{\mathbf{k}}$ is the one-body lattice Hamiltonian, μ is the chemical potential, $\mathbf{I}$ is the identity matrix in orbital-spin space, and N_k is the number of $\mathbf{k}$ -points in the Brillouin zone. After the DMFT mapping, we must solve an impurity problem whose Green's function and self-energy coincide with the local lattice quantities at self-consistency:

$$\mathbf{G}_{\text{imp}}(i\omega_n) = \mathbf{G}_{\text{loc}}(i\omega_n), \quad \Sigma_{\text{imp}}(i\omega_n) = \Sigma_{\text{latt}}(i\omega_n). \quad (3.3)$$

The impurity problem is completely specified by the local Hamiltonian H_{loc} and the hybridization function $\Delta(i\omega_n)$. H_{loc} describes the local physics of the lattice, and is generally given by

$$H_{\text{loc}} = \sum_{\alpha\gamma}^n \varepsilon_{\alpha\gamma} c_{\alpha}^{\dagger} c_{\gamma} + \sum_{\alpha\gamma\delta\nu}^n U_{\alpha\gamma\delta\nu} c_{\alpha}^{\dagger} c_{\gamma}^{\dagger} c_{\delta} c_{\nu}, \quad (3.4)$$

where $c_{\alpha}^{\dagger}$ (c_{α}) create (annihilate) an electron in the impurity orbital-spin flavor α , n is the number of impurity flavors, and $\varepsilon_{\alpha\gamma}$ and $U_{\alpha\gamma\delta\nu}$ are the local one-body and two-body contributions, respectively. The hybridization function $\Delta(i\omega_n)$ satisfies the Dyson equation

$$\Delta(i\omega_n) = (i\omega_n - \mu) \mathbf{I} - \varepsilon - \Sigma_{\text{latt}}(i\omega_n) - \mathbf{G}_{\text{loc}}^{-1}(i\omega_n), \quad (3.5)$$

The Anderson impurity model (AIM) action is then given in imaginary time by

$$\begin{aligned} S_{\text{AIM}} = & \int_0^{\beta} d\tau \sum_{\alpha}^n c_{\alpha}^{\dagger}(\tau) \partial_{\tau} c_{\alpha}(\tau) + \int_0^{\beta} d\tau H_{\text{loc}}[c_{\alpha}^{\dagger}, c_{\alpha}] \\ & + \int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{\alpha\gamma}^n c_{\alpha}^{\dagger}(\tau) \Delta_{\alpha\gamma}(\tau - \tau') c_{\gamma}(\tau'). \end{aligned} \quad (3.6)$$

The atomic limit corresponds to $\Delta(i\omega_n) = 0$: the impurity is decoupled from its environment and the problem reduces to the diagonalization of H_{loc} . A finite hybridization function describes virtual hopping processes between the impurity and the bath, and therefore controls the deviation from the atomic limit. This makes $\Delta(i\omega_n)$ a natural parameter for a perturbative expansion in a strong-coupling impurity solver.

3.1.1 Pseudoparticle representation

We follow the approach of Refs. [97–99]: in order to treat the hybridization term in the impurity action perturbatively, we enlarge the Hilbert space of the impurity problem so that the hybridization term of the action (3.6) becomes quartic in the new degrees of freedom, and then employ standard perturbation theory. The enlarged space will be the auxiliary Fock space of pseudoparticles $\mathcal{H}_{\text{pp}}$. We denote the original impurity Hilbert space by $\mathcal{H}_{\text{imp}}$, and choose a complete many-body basis of this space, denoted $\{|m\rangle\}_{m=1}^N$ with $N = 2^n$. In what follows, operators with a symbol $\hat{\cdot}$ act on the space $\mathcal{H}_{\text{pp}}$, whereas operators without this symbol act on the original impurity Hilbert space $\mathcal{H}_{\text{imp}}$.

For each basis state $|m\rangle \in \mathcal{H}_{\text{imp}}$, we introduce pseudoparticle creation and annihilation operators $\hat{p}_m^\dagger$ and $\hat{p}_m$ on $\mathcal{H}_{\text{pp}}$. We also introduce a normalized pseudoparticle vacuum state $|\text{vac}\rangle$ such that $\hat{p}_m |\text{vac}\rangle = 0$ for all m . Finally, we define the pseudoparticle commutation relations given by the following rule: if the state $|m\rangle$ contains an even number of electrons (N_m), $\hat{p}_m$ is bosonic, and if $|m\rangle$ contains an odd number of electrons, $\hat{p}_m$ is fermionic. Equivalently,

$$\begin{aligned} \hat{p}_m \hat{p}_n^\dagger - \zeta_{mn} \hat{p}_n^\dagger \hat{p}_m &= \delta_{mn}, & \zeta_{mn} &= (-1)^{N_m N_n}. \\ \hat{p}_m \hat{p}_n - \zeta_{mn} \hat{p}_n \hat{p}_m &= 0, \end{aligned} \quad (3.7)$$

The reason for this choice of commutation relations will become clear below.

With these definitions, the pseudoparticle Fock space $\mathcal{H}_{\text{pp}}$ is the closure of the span of all states obtained by acting on the vacuum state $|\text{vac}\rangle$ with products of the pseudoparticle creation operators $\hat{p}_m^\dagger$, i.e., the states $|\Psi\rangle = \prod_{m=1}^N (\hat{p}_m^\dagger)^{n_m} |\text{vac}\rangle$, with the following constraint: n_m can only be 0 or 1 if $\hat{p}_m$ is fermionic (i.e., if $|m\rangle$ contains an odd number of electrons), while n_m can be any non-negative integer if $\hat{p}_m$ is bosonic (i.e., if $|m\rangle$ contains an even number of electrons).

We associate the impurity many-body states $|m\rangle$ with the single-pseudoparticle states $|m\rangle_{\text{pp}} = \hat{p}_m^\dagger |\text{vac}\rangle$. Thus, the original impurity Hilbert space $\mathcal{H}_{\text{imp}}$ is embedded in the pseudoparticle Fock space $\mathcal{H}_{\text{pp}}$, i.e., the impurity many-body states are the single-pseudoparticle states in $\mathcal{H}_{\text{pp}}$. We refer to the subspace spanned by the single-pseudoparticle states $|m\rangle_{\text{pp}}$ as the physical subspace $\mathcal{H}_{\text{phys}}$, and have $\mathcal{H}_{\text{imp}} \cong \mathcal{H}_{\text{phys}} \subset \mathcal{H}_{\text{pp}}$. Equivalently, defining the pseudoparticle number operator

$$\hat{Q} \equiv \sum_{m=1}^N \hat{p}_m^\dagger \hat{p}_m, \quad (3.8)$$

it can be shown that $\mathcal{H}_{\text{phys}}$ is the $Q = 1$ eigenspace of $\hat{Q}$,

$$\mathcal{H}_{\text{phys}} = \{|\Psi\rangle \in \mathcal{H}_{\text{pp}} \mid \hat{Q} |\Psi\rangle = |\Psi\rangle\}. \quad (3.9)$$

Sectors with $Q = 0$ or $Q > 1$ are artifacts of the enlarged Hilbert space and must be projected out when computing physical quantities.

We now consider the extension of the impurity creation and annihilation operators $c_\alpha^\dagger$ and c_α from $\mathcal{H}_{\text{imp}}$ to operators $\hat{c}_\alpha^\dagger$ and $\hat{c}_\alpha$ on $\mathcal{H}_{\text{pp}}$. We posit the bilinear representation

$$\begin{aligned}\hat{c}_\alpha &= \sum_{mn} F_{mn}^\alpha \hat{p}_m^\dagger \hat{p}_n, \\ \hat{c}_\alpha^\dagger &= \sum_{mn} (F_{nm}^\alpha)^* \hat{p}_m^\dagger \hat{p}_n,\end{aligned}\tag{3.10}$$

where $F_{mn}^\alpha = \langle m | c_\alpha | n \rangle$ are the matrix elements of the original impurity operators. It follows from (3.7) that

$$\hat{c}_\alpha |n\rangle_{\text{pp}} = \sum_m F_{mn}^\alpha |m\rangle_{\text{pp}},\tag{3.11}$$

and acting from the left with $\langle k |_{\text{pp}}$ shows that the matrix elements of $\hat{c}_\alpha$ within $\mathcal{H}_{\text{phys}}$ coincide with those of c_α in $\mathcal{H}_{\text{imp}}$. Thus (3.10) gives the proper extension of the impurity field operators to $\mathcal{H}_{\text{pp}}$. We now show that the particular choice of commutation relations (3.7) ensures that the extended operators $\hat{c}_\alpha$ and $\hat{c}_\alpha^\dagger$ satisfy the canonical anticommutation relations of fermionic operators within $\mathcal{H}_{\text{phys}}$,

$$\{\hat{c}_\alpha, \hat{c}_\gamma^\dagger\} = \delta_{\alpha\gamma}, \quad \{\hat{c}_\alpha, \hat{c}_\gamma\} = \{\hat{c}_\alpha^\dagger, \hat{c}_\gamma^\dagger\} = 0.\tag{3.12}$$

We first note that the matrix elements $F_{mn}^\alpha = \langle m | c_\alpha | n \rangle$ are nonzero only if $N_m = N_n - 1$, i.e., only if the states $|m\rangle$ and $|n\rangle$ have opposite electron number parity. Using the bilinear representation (3.10), we have

$$\{\hat{c}_\alpha, \hat{c}_\gamma^\dagger\} = \sum_{mnkl} F_{mn}^\alpha (F_{lk}^\gamma)^* \{\hat{p}_m^\dagger \hat{p}_n, \hat{p}_k^\dagger \hat{p}_l\},\tag{3.13a}$$

$$\{\hat{c}_\alpha, \hat{c}_\gamma\} = \sum_{mnkl} F_{mn}^\alpha F_{kl}^\gamma \{\hat{p}_m^\dagger \hat{p}_n, \hat{p}_k^\dagger \hat{p}_l\}.\tag{3.13b}$$

The commutation relations (3.7) give

$$\begin{aligned}(\hat{p}_m^\dagger \hat{p}_n)(\hat{p}_k^\dagger \hat{p}_l) &= \zeta_{nk} \zeta_{mk} \zeta_{nl} \hat{p}_k^\dagger \hat{p}_m^\dagger \hat{p}_l \hat{p}_n + \delta_{nk} \hat{p}_m^\dagger \hat{p}_l, \\ (\hat{p}_k^\dagger \hat{p}_l)(\hat{p}_m^\dagger \hat{p}_n) &= \zeta_{lm} \hat{p}_k^\dagger \hat{p}_m^\dagger \hat{p}_l \hat{p}_n + \delta_{lm} \hat{p}_k^\dagger \hat{p}_n.\end{aligned}\tag{3.14}$$

Note that

$$\begin{aligned}(\zeta_{nk} \zeta_{mk} \zeta_{nl} + \zeta_{lm}) \zeta_{lm} &= \zeta_{nk} \zeta_{mk} \zeta_{nl} \zeta_{lm} + \zeta_{lm}^2 \\ &= (-1)^{(N_m + N_n)(N_k + N_l)} + 1 = 0,\end{aligned}\tag{3.15}$$

since $N_m + N_n$ and $N_k + N_l$ are both odd in the non-zero terms of (3.13). Since $\zeta_{lm} = \pm 1$, this implies $\zeta_{nk} \zeta_{mk} \zeta_{nl} + \zeta_{lm} = 0$, so (3.14) yields

$$\{\hat{p}_m^\dagger \hat{p}_n, \hat{p}_k^\dagger \hat{p}_l\} = \delta_{nk} \hat{p}_m^\dagger \hat{p}_l + \delta_{lm} \hat{p}_k^\dagger \hat{p}_n.\tag{3.16}$$

Substituting (3.16) into (3.13a) yields

$$\{\hat{c}_\alpha, \hat{c}_\gamma^\dagger\} = \sum_{mnl} F_{mn}^\alpha (F_{ln}^\gamma)^* \hat{p}_m^\dagger \hat{p}_l + \sum_{mnk} F_{mn}^\alpha (F_{mk}^\gamma)^* \hat{p}_k^\dagger \hat{p}_n.\tag{3.17}$$

Recognizing that $\sum_n F_{mn}^\alpha (F_{ln}^\gamma)^* = \langle m | c_\alpha c_\gamma^\dagger | l \rangle$ and $\sum_m F_{mn}^\alpha (F_{mk}^\gamma)^* = \langle k | c_\gamma^\dagger c_\alpha | n \rangle$, and relabeling indices in the second term, we obtain

$$\begin{aligned} \{\hat{c}_\alpha, \hat{c}_\gamma^\dagger\} &= \sum_{ml} \langle m | \{c_\alpha, c_\gamma^\dagger\} | l \rangle \hat{p}_m^\dagger \hat{p}_l \\ &= \delta_{\alpha\gamma} \sum_m \hat{p}_m^\dagger \hat{p}_m = \delta_{\alpha\gamma} \hat{Q}, \end{aligned} \quad (3.18)$$

which is the first of the relations (3.12) once we notice that $\hat{Q} = 1$ in the physical subspace $\mathcal{H}_{\text{phys}}$. Similarly, one finds $\{\hat{c}_\alpha, \hat{c}_\gamma\} = \sum_{ml} \langle m | \{c_\alpha, c_\gamma\} | l \rangle \hat{p}_m^\dagger \hat{p}_l = 0$, completing the proof.

We are now prepared to extend the impurity action in Eq. (3.6) to the pseudoparticle space $\mathcal{H}_{\text{pp}}$ by replacing the impurity field operators with their extensions (3.10):

$$\begin{aligned} \hat{S}_{\text{imp}} &= \int_0^\beta d\tau \sum_m \hat{p}_m^\dagger(\tau) \partial_\tau \hat{p}_m(\tau) + \int_0^\beta d\tau \sum_{mn} \hat{p}_m^\dagger(\tau) \langle m | H_{\text{loc}} | n \rangle \hat{p}_n(\tau) \\ &\quad + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{mni j} \hat{p}_m^\dagger(\tau) \hat{p}_n(\tau) \left(\sum_{\alpha\gamma} (F_{nm}^\alpha)^* \Delta_{\alpha\gamma}(\tau - \tau') F_{ij}^\gamma \right) \hat{p}_i^\dagger(\tau') \hat{p}_j(\tau'). \end{aligned} \quad (3.19)$$

The first two terms describe the propagation of atomic many-body states and are quadratic in the pseudoparticle operators. The last term originates from the hybridization function and is quartic in the pseudoparticle operators. This structure makes the atomic limit the natural unperturbed reference point and the hybridization the expansion parameter. The non-crossing approximation (NCA) is the lowest-order approximation in this strong-coupling expansion, retaining the simplest skeleton diagrams for the pseudoparticle self-energy. Systematic corrections are obtained by including diagrams with additional hybridization lines and crossings. The resulting crossing expansion, which we refer to as XCA, has been described in detail in Refs. [42, 43]; here we only summarize the ingredients needed for the calculation of static and dynamical observables.

3.2 Computing physical quantities

We next discuss how to compute the impurity partition function and the expectation values of physical observables within the pseudoparticle representation. A key practical advantage of this approach is that the partition function is obtained explicitly, so that observables and thermodynamic potentials follow directly from it. Monte Carlo techniques, by contrast, sample only the normalized Boltzmann weights and therefore do not access the partition function itself, forcing quantities such as the free energy and the entropy to be reconstructed indirectly through a thermodynamic integration. In this section we will not address how to evaluate the single-particle Green's function from the pseudoparticle propagators, this has been discussed in detail in Refs. [42, 43].

In the following it is convenient to adopt a Hamiltonian formulation of the impurity problem, equivalent to the action (3.6), in which the bath degrees of freedom are reintroduced explicitly. The hybridization function can be generated by coupling the impurity site to a set of non-interacting fermionic levels $f_{b\mathbf{k}}$, leading to the AIM Hamiltonian

$$H_{\text{AIM}} = H_{\text{loc}} + \sum_{\alpha b \mathbf{k}} (V_{\alpha b \mathbf{k}} c_{\alpha}^{\dagger} f_{b \mathbf{k}} + \text{H.c.}) + \sum_{b \mathbf{k}} \epsilon_{b \mathbf{k}} f_{b \mathbf{k}}^{\dagger} f_{b \mathbf{k}}. \quad (3.20)$$

Here $f_{b \mathbf{k}}^{\dagger}$ creates an electron of energy $\epsilon_{b \mathbf{k}}$ in the level $\mathbf{k}$ of the bath channel b , and the $V_{\alpha b \mathbf{k}}$ are hybridization amplitudes. Integrating out the f electrons reproduces the hybridization term of (3.6) provided that

$$\Delta_{\alpha \gamma}(i\omega_n) = \sum_{b \mathbf{k}} \frac{V_{\alpha b \mathbf{k}} V_{\gamma b \mathbf{k}}^*}{i\omega_n - \epsilon_{b \mathbf{k}}}, \quad (3.21)$$

which is the condition fixing the bath parameters in terms of the hybridization function (3.5). We emphasize that in the following formal manipulations the bath partition function will drop out of the physical observables, so that no explicit set of bath parameters ever needs to be determined.

In the pseudoparticle formulation we replace the impurity operators c_{α} and $c_{\alpha}^{\dagger}$ in H_{AIM} by their bilinear representations, and denote the resulting operator acting on $\mathcal{H}_{\text{pp}} \otimes \mathcal{H}_{\text{bath}}$ by $\hat{H}_{\text{AIM}}$.

According to (3.9), physical averages must be computed in the physical subspace,

$$\langle \hat{\mathcal{O}} \rangle_{\text{phys}} = \frac{\sum_{|\psi\rangle \in \mathcal{H}_{\text{phys}} \otimes \mathcal{H}_{\text{bath}}} \langle \psi | e^{-\beta \hat{H}_{\text{AIM}}} \hat{\mathcal{O}} | \psi \rangle}{\sum_{|\psi\rangle \in \mathcal{H}_{\text{phys}} \otimes \mathcal{H}_{\text{bath}}} \langle \psi | e^{-\beta \hat{H}_{\text{AIM}}} | \psi \rangle}. \quad (3.22)$$

Directly restricting all traces to this sector is possible in principle, but it is more convenient to implement the projection by introducing a Lagrange multiplier λ conjugate to $\hat{Q}$ and working in the resulting grand-canonical ensemble. Only at the end we take the limit $\lambda \rightarrow \infty$ to project onto the physical subspace.

We first define the grand-canonical partition function

$$Z_G(\lambda) = \text{Tr}_G \left(e^{-\beta(\hat{H}_{\text{AIM}} + \lambda \hat{Q})} \right) \equiv \sum_{|\psi\rangle \in \mathcal{H}_{\text{pp}} \otimes \mathcal{H}_{\text{bath}}} \langle \psi | e^{-\beta(\hat{H}_{\text{AIM}} + \lambda \hat{Q})} | \psi \rangle. \quad (3.23)$$

Then we define the canonical partition function restricted to the sector with pseudoparticle number Q as

$$Z_C(Q) = \text{Tr}_Q \left(e^{-\beta \hat{H}_{\text{AIM}}} \right) \equiv \sum_{\substack{|\psi\rangle \in \mathcal{H}_{\text{pp}} \otimes \mathcal{H}_{\text{bath}} \\ \hat{Q}|\psi\rangle = Q|\psi\rangle}} \langle \psi | e^{-\beta \hat{H}_{\text{AIM}}} | \psi \rangle \quad (3.24)$$

We now observe that in the $Q = 0$ sector all terms in $\hat{H}_{\text{AIM}}$ involving the pseudoparticles operators vanish. Thus, only the free bath Hamiltonian of the $f_{b \mathbf{k}}$ contributes non-

trivially to the trace in $Z_C(0)$, and we obtain the partition function of the bath only,

$$\begin{aligned} Z_C(0) &= \text{Tr}_{Q=0} \left(e^{-\beta \hat{H}_{\text{AIM}}} \right) \\ &= \sum_{|\psi\rangle \in \mathcal{H}_{\text{bath}}} \langle \psi | e^{-\beta \sum_{b\mathbf{k}} \epsilon_{b\mathbf{k}} f_{b\mathbf{k}}^\dagger f_{b\mathbf{k}}} | \psi \rangle \\ &\equiv Z_{\text{bath}}. \end{aligned} \quad (3.25)$$

Similarly, it follows from its definition that $Z_C(1)$ corresponds to the partition function of the AIM restricted to the physical subspace $\mathcal{H}_{\text{phys}}$ of the pseudoparticle Fock space, and therefore coincides with the physical AIM partition function

$$Z_C(1) = \sum_{|\psi\rangle \in \mathcal{H}_{\text{phys}} \otimes \mathcal{H}_{\text{bath}}} \langle \psi | e^{-\beta \hat{H}_{\text{AIM}}} | \psi \rangle \equiv Z_{\text{AIM}} \quad (3.26)$$

Now, since $\hat{Q}$ is a conserved quantity ($[\hat{H}_{\text{AIM}}, \hat{Q}] = 0$), we can decompose the trace in $Z_G(\lambda)$ into sectors of fixed pseudoparticle number,

$$\begin{aligned} Z_G(\lambda) &= \sum_{Q=0}^{\infty} e^{-\beta \lambda Q} \text{Tr}_Q \left(e^{-\beta \hat{H}_{\text{AIM}}} \right) \\ &\equiv \sum_{Q=0}^{\infty} \xi^Q Z_C(Q), \end{aligned} \quad (3.27)$$

where we have defined $\xi \equiv e^{-\beta \lambda}$ the fugacity associated to the pseudoparticle number. The expectation value of the pseudoparticle number in the grand-canonical ensemble is therefore

$$\langle \hat{Q} \rangle_\lambda = \frac{1}{Z_G(\lambda)} \sum_{Q=1}^{\infty} Z_C(Q) Q \xi^Q, \quad (3.28)$$

which we can rewrite as

$$\xi^{-1} \langle \hat{Q} \rangle_\lambda Z_G(\lambda) = \sum_{Q=1}^{\infty} Q Z_C(Q) \xi^{Q-1} = Z_C(1) + \mathcal{O}(\xi). \quad (3.29)$$

Taking now the limit $\lambda \rightarrow \infty$ of the above expressions (3.27) and (3.29), we obtain

$$\begin{aligned} \lim_{\lambda \rightarrow \infty} Z_G(\lambda) &= Z_C(0), \\ \lim_{\lambda \rightarrow \infty} \xi^{-1} \langle \hat{Q} \rangle_\lambda Z_G(\lambda) &= Z_C(1) = Z_{\text{AIM}}, \end{aligned} \quad (3.30)$$

thus

$$Z_{\text{AIM}} = Z_C(0) \lim_{\lambda \rightarrow \infty} \xi^{-1} \langle \hat{Q} \rangle_\lambda. \quad (3.31)$$

Given now the physical AIM partition function Z_{AIM} , we can readily evaluate the expectation value of any operator $\hat{\mathcal{O}}$ in the physical subspace (3.22) as

$$\langle \hat{\mathcal{O}} \rangle_{\text{phys}} = \frac{\text{Tr}_{Q=1} \left(e^{-\beta \hat{H}_{\text{AIM}}} \hat{\mathcal{O}} \right)}{Z_{\text{AIM}}} \quad (3.32)$$

Next, we observe that

$$\begin{aligned} \langle \hat{\mathcal{O}} \hat{Q} \rangle_\lambda &= \frac{1}{Z_G(\lambda)} \sum_{Q=0}^{\infty} \text{Tr}_Q \left(e^{-\beta \hat{H}_{\text{AIM}}} \hat{\mathcal{O}} \right) Q e^{-\beta \lambda Q} \\ &\xrightarrow{\lambda \rightarrow \infty} \frac{\xi}{Z_C(0)} \text{Tr}_{Q=1} \left(e^{-\beta \hat{H}_{\text{AIM}}} \hat{\mathcal{O}} \right) \end{aligned} \quad (3.33)$$

or equivalently

$$\lim_{\lambda \rightarrow \infty} \left(\langle \hat{\mathcal{O}} \hat{Q} \rangle_\lambda Z_C(0) \xi^{-1} \right) = \text{Tr}_{Q=1} (e^{-\beta \hat{H}_{\text{AIM}}} \hat{\mathcal{O}}) \quad (3.34)$$

Inserting now (3.31) and (3.34) into the definition of the physical expectation value (3.32), we obtain

$$\langle \hat{\mathcal{O}} \rangle_{\text{phys}} = \lim_{\lambda \rightarrow \infty} \left(\frac{\langle \hat{\mathcal{O}} \hat{Q} \rangle_\lambda}{\langle \hat{Q} \rangle_\lambda} \right) \quad (3.35)$$

If, as it's usually the case, we are interested in the expectation value of a physical observable, this is by definition zero in the $Q = 0$ sector and the leading in λ term in the expansion of $\langle \hat{\mathcal{O}} \hat{Q} \rangle_\lambda$ is $\langle \hat{\mathcal{O}} \rangle_\lambda$. Therefore, we can drop the $\hat{Q}$ operator in the numerator of the above expression

$$\langle \hat{\mathcal{O}} \rangle_{\text{phys}} = \lim_{\lambda \rightarrow \infty} \left(\frac{\langle \hat{\mathcal{O}} \rangle_\lambda}{\langle \hat{Q} \rangle_\lambda} \right) \quad (3.36)$$

We need now a recipe to evaluate the expectation values $\langle \hat{\mathcal{O}} \rangle_\lambda$ and $\langle \hat{Q} \rangle_\lambda$ in the grand-canonical ensemble and take their $\lambda \rightarrow \infty$ limit. To do that, we define the single-pseudoparticle Green's function in the grand-canonical ensemble

$$\begin{aligned} \mathcal{G}_{mn}^\lambda(\tau) &\equiv -\langle T_\tau \{ \hat{p}_m^\lambda(\tau) \hat{p}_n^{\lambda\dagger}(0) \} \rangle_\lambda \\ &= -\frac{1}{Z_G(\lambda)} \text{Tr} \left(e^{-\beta(\hat{H}_{\text{AIM}} + \lambda \hat{Q})} T_\tau \{ \hat{p}_m^\lambda(\tau) \hat{p}_n^{\lambda\dagger}(0) \} \right), \end{aligned} \quad (3.37)$$

with the time-evolved operators

$$\hat{p}_m^\lambda(\tau) = e^{\tau(\hat{H}_{\text{AIM}} + \lambda \hat{Q})} \hat{p}_m e^{-\tau(\hat{H}_{\text{AIM}} + \lambda \hat{Q})}. \quad (3.38)$$

Evaluating the pseudoparticle Green's function at $\tau = \beta$ and tracing over the pseudoparticle indices we get

$$\begin{aligned} -\sum_m \mathcal{G}_{mm}^\lambda(\tau = \beta) &= \frac{1}{Z_G(\lambda)} \text{Tr} \left(e^{-\beta(\hat{H}_{\text{AIM}} + \lambda \hat{Q})} \sum_m \hat{p}_m^\dagger \hat{p}_m \right) \\ &= \langle \hat{Q} \rangle_\lambda \end{aligned} \quad (3.39)$$

Similarly, for a generic operator $\hat{\mathcal{O}} = \sum_{mn} \mathcal{O}_{mn} \hat{p}_m^\dagger \hat{p}_n$ we can write

$$\langle \hat{\mathcal{O}} \rangle_\lambda = -\sum_{mn} \mathcal{O}_{mn} \mathcal{G}_{nm}^\lambda(\tau = \beta) \quad (3.40)$$

Now we observe that the time-evolved pseudoparticle operators satisfy

$$\begin{aligned}\partial_\lambda \hat{p}_i^\lambda(\tau) &= e^{\tau(\hat{H}_{\text{AIM}} + \lambda \hat{Q})} [\tau \hat{Q}, \hat{p}_i] e^{-\tau(\hat{H}_{\text{AIM}} + \lambda \hat{Q})} \\ &= -\tau \hat{p}_i^\lambda(\tau)\end{aligned}\tag{3.41}$$

and thus

$$\hat{p}_i^\lambda(\tau) = e^{-\lambda\tau} \hat{p}_i(\tau) \quad \text{with} \quad \hat{p}_i(\tau) = e^{\tau \hat{H}_{\text{AIM}}} \hat{p}_i e^{-\tau \hat{H}_{\text{AIM}}}\tag{3.42}$$

Expanding at the lowest order in the fugacity ξ the pseudoparticle Green's function we get

$$\begin{aligned}\mathcal{G}_{mn}^\lambda(\tau) &= -\frac{1}{Z_G(\lambda)} \sum_{Q=0}^{\infty} e^{-\lambda\tau} \text{Tr}_Q \left(e^{-\beta \hat{H}_{\text{AIM}}} T_\tau \{ \hat{p}_m(\tau) \hat{p}_n^\dagger(0) \} \right) e^{-\beta \lambda Q} \\ &\xrightarrow{\lambda \rightarrow \infty} -\frac{e^{-\lambda\tau}}{Z_C(0)} \text{Tr}_{Q=0} \left(e^{-\beta \hat{H}_{\text{AIM}}} T_\tau \{ \hat{p}_m(\tau) \hat{p}_n^\dagger(0) \} \right) \\ &\equiv e^{-\lambda\tau} \mathcal{G}_{mn}(\tau)\end{aligned}\tag{3.43}$$

where the *projected Green's function* $\mathcal{G}_{mn}(\tau)$ is independent of λ and it's the building block in the diagrammatic expansion implemented in the XCA algorithm. Once it is known, the expectation value of a physical operator can be obtained as

$$\langle \hat{\mathcal{O}} \rangle_{\text{phys}} = \frac{\sum_{mn} \mathcal{O}_{mn} \mathcal{G}_{nm}(\tau = \beta)}{\sum_m \mathcal{G}_{mm}(\tau = \beta)}\tag{3.44}$$

In the remainder of this chapter, we therefore treat XCA as the numerical backend that supplies the projected pseudoparticle Green's function, together with the energy shifts introduced below, and focus on how these quantities yield physical observables and thermodynamic potentials. Further details of the diagrammatic expansion and its numerical implementation can be found in Refs. [42, 43].

3.2.1 Impurity and lattice free energies

We conclude this section discussing how to compute the free energy of the impurity site once the bath contribution has been traced out, and then the related free energy of the original lattice within DMFT. First, we notice that to compute $\mathcal{G}_{mn}(\tau)$, we have to solve the equations of motion that govern its time evolution [43]. In absence of hybridization, the atomic $\mathcal{G}_{mn}^0(\tau)$ satisfies

$$(-\partial_\tau - \hat{H}_{\text{loc}}) \mathcal{G}^0(\tau) = 0, \quad \mathcal{G}^0(0) = -\mathbb{I}\tag{3.45}$$

When we switch on the hybridization, $\mathcal{G}_{mn}(\tau)$ obeys

$$(-\partial_\tau - \hat{H}_{\text{imp}} - \Sigma*) \mathcal{G}(\tau) = 0, \quad \mathcal{G}(0) = -\mathbb{I}\tag{3.46}$$

where Σ is the pseudoparticle self-energy, and the $*$ denotes a convolution in imaginary time

$$(\Sigma * \mathcal{G})(\tau) = \int_0^\tau d\tau' \Sigma(\tau - \tau') \mathcal{G}(\tau').\tag{3.47}$$

Given the solution of this equation of motion we can easily get the free energy of the impurity site f_{imp} tracing out the bath degrees of freedom from the AIM partition function

$$\begin{aligned} e^{-\beta f_{\text{imp}}} &= \frac{Z_{\text{AIM}}}{Z_C(0)} \\ &= \lim_{\lambda \rightarrow \infty} e^{\beta \lambda} \langle \hat{Q} \rangle_\lambda \\ &= - \sum_m \mathcal{G}_{mm}(\tau = \beta) \end{aligned} \quad (3.48)$$

It's now important to highlight a subtle point: It's standard recipe, as implemented in the XCA algorithm, to introduce energy shifts in the equations of motion to improve their numerical stability. To properly extract the free energy, we must account for these shifts. The shifted equation of motion for the atomic projected Green's function reads

$$(-\partial_\tau - \hat{H}_{\text{loc}} - \eta_0) \tilde{\mathcal{G}}^0(\tau) = 0, \quad \tilde{\mathcal{G}}^0(0) = -\mathbb{I} \quad (3.49)$$

where the shifted atomic projected Green's function $\tilde{\mathcal{G}}^0(\tau)$ is related to the unshifted one by

$$\tilde{\mathcal{G}}^0(\tau) = e^{-\eta_0 \tau} \mathcal{G}^0(\tau) \quad (3.50)$$

and η_0 is chosen to normalize the atomic partition function to 1:

$$e^{-\beta \tilde{f}_{\text{imp}}^0} = - \sum_m \tilde{\mathcal{G}}_{mm}^0(\tau = \beta) = 1 \quad (3.51)$$

Similarly, the equation of motion for the fully interacting projected pseudoparticle Green's function is shifted with respect to Eq. (3.46):

$$(-\partial_\tau - \hat{H}_{\text{imp}} - (\eta_0 + \eta) - \Sigma^*) \tilde{\mathcal{G}}(\tau) = 0, \quad \tilde{\mathcal{G}}(0) = -\mathbb{I} \quad (3.52)$$

where η is an additional shift introduced to further improve the numerical stability by also normalizing the fully interacting partition function of the impurity site. The relation between the shifted and unshifted projected pseudoparticle propagators reads again

$$\tilde{\mathcal{G}}(\tau) = e^{-(\eta_0 + \eta)\tau} \mathcal{G}(\tau) \quad (3.53)$$

with a shifted impurity free energy

$$\begin{aligned} e^{-\beta \tilde{f}_{\text{imp}}} &= - \sum_m \tilde{\mathcal{G}}_{mm}(\tau = \beta) \\ &= e^{-\beta(\eta_0 + \eta)} e^{-\beta f_{\text{imp}}} = 1 \end{aligned} \quad (3.54)$$

Accounting for these shifts, the physical unshifted impurity site free energy is simply given as

$$f_{\text{imp}} = -(\eta_0 + \eta) \quad (3.55)$$

where η_0 is fixed by the atomic Hamiltonian

$$\eta_0 = \frac{1}{\beta} \ln \left(\text{Tr} e^{-\beta \hat{H}_{\text{loc}}} \right) \quad (3.56)$$

while η is determined self-consistently during the solution of the equations of motion and it's provided in the output of the XCA solver.

Once the impurity site free energy is computed, the lattice free energy per site can be obtained by exploiting the Luttinger-Ward functional $\Phi[G, U]$ [26]. The Luttinger-Ward functional is a functional of the Green's function and the interaction parameters, and it encodes the many-body effects of the system. Within the DMFT approximation, the lattice free energy per site can be expressed in terms of the impurity free energy and the local density of states $\mathbf{D}(\omega) = -1/\pi \text{Im } \mathbf{G}_{\text{loc}}(\omega + i0^+)$ as

$$f_{\text{latt}} = f_{\text{imp}} - T \sum_n \int_{-\infty}^{+\infty} d\omega \text{Tr} \left[\mathbf{D}(\omega) \ln((i\omega_n + \mu - \omega) \mathbf{I} - \Sigma(i\omega_n)) + \ln \mathbf{G}_{\text{loc}}(i\omega_n) \right] \quad (3.57)$$

with ω a real frequency.

3.3 Results on the single-band Hubbard model

In this section we discuss the results obtained with the XCA algorithm on the single-band Hubbard model on the Bethe lattice, a paradigmatic model for strongly correlated electron systems. We focus on the low-temperature regime, where the system undergoes a metal-Mott insulator (MI) transition once the onset of antiferromagnetism is precluded.

The model Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}, \quad (3.58)$$

with t the hopping amplitude between nearest-neighbor sites i and j , U the local interaction strength, μ the chemical potential, $c_{i\sigma}^\dagger$ the creation operator for an electron with spin σ at site i , and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ the number operator. For the Bethe lattice, we use the noninteracting density of states

$$D(\omega) = \frac{2}{\pi D^2} \sqrt{D^2 - \omega^2}, \quad |\omega| \leq D, \quad (3.59)$$

and half-bandwidth $D = 2$ throughout, so that $t = D/2 = 1$. The results discussed in this section have been obtained with the following XCA parameters (see [42, 43]): $\epsilon^{\text{DLR}} = 10^{-7}$, the target accuracy of the DLR representation of the imaginary-time propagators; $\omega_{\text{max}}^{\text{DLR}} = 10$, the frequency cutoff on the spectral densities entering the DLR representations; $\epsilon^{\text{pp-solver}} = 10^{-6}$, the convergence threshold on the pseudoparticle Green's function self-consistency. The DMFT loop is instead converged until the difference between two consecutive iterations of the hybridization function is smaller than 10^{-5} for every τ in the imaginary time grid.

To assess the accuracy with the expansion order of our calculations, we benchmark them with a reference solution obtained by solving the impurity problem with the

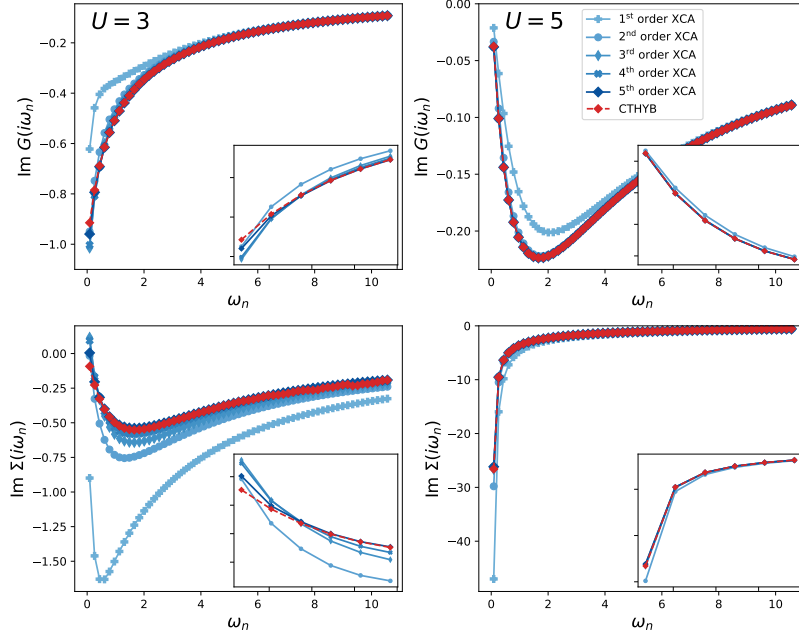


Figure 3.1: Matsubara Green’s function $G(i\omega_n)$ and self-energy $\Sigma(i\omega_n)$ for the half-filled Hubbard model in the metallic ($U = 3$) and Mott insulating ($U = 5$) solutions. Only the imaginary part of the Green’s function and self-energy is shown, as the real part is zero by particle-hole symmetry. The insets zoom on the first 6 positive Matsubara frequencies.

continuous-time hybridization expansion (CTHYB) solver implemented in the TRIQS library [72, 73, 92, 93, 100–102]. The statistical accuracy of the reference solution is estimated by solving the same impurity problem ten times independently on the converged DMFT hybridization bath and computing the standard deviation of the resulting self-energy across Matsubara frequencies; the same procedure is used for the static observables.

3.3.1 Dynamical Green’s function

We first examine the dynamical properties of the half-filled system, i.e. one electron per site on average. In Fig. 3.1 we show the Matsubara Green’s function and self-energy for two representative values of the interaction strength U : one corresponding to a metallic solution ($U = 3$) and one corresponding to an insulating solution ($U = 5$). The inverse temperature is set to $\beta = 36$, corresponding to half the critical temperature of the metal-MI transition [103, 104], therefore in the low-temperature regime. The XCA method is able to capture both the metallic and insulating solutions, but the convergence with the expansion order is much faster in the insulating case, where the solution is adiabatically connected to the atomic limit. Looking at the first, fifth, and fifteenth Matsubara frequencies, Fig. 3.2 shows that the self-energy converges uniformly in the insulating case, approaching the reference solution (obtained with $N_{\text{cycles}} = 10^7$ MC measurements) within the estimated accuracy of the MC sampling already at the

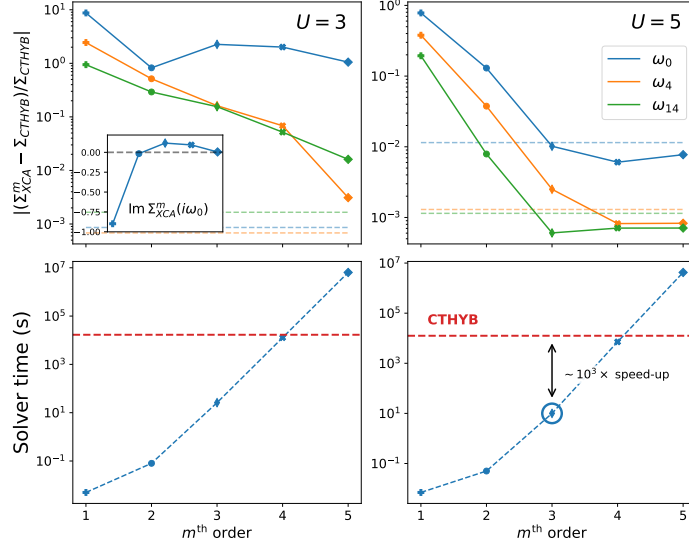


Figure 3.2: Top panels: Relative error on the self-energy $\Sigma(i\omega_n)$ with respect to the reference solution for the metal ($U = 3$) and Mott insulator ($U = 5$) at $\beta = 36$. The horizontal dashed lines indicate the estimated relative accuracy of the CTHYB reference solution, computed as the standard deviation over ten independent runs. In the inset of the top-left panel, we show the imaginary part of the self-energy at the first Matsubara frequency, which develops a non-physical positive value improving non-monotonically with the expansion order. Bottom panels: Timings (in seconds) for a single impurity solution within a DMFT iteration as a function of the expansion order.

third expansion order. On the other hand, in the metallic case the convergence is much slower, especially at low frequencies. This behavior is expected: within NCA, i.e. 1st-order expansion (and in its higher-order extensions that retain only a finite number of skeleton diagrams for the self-energy), the low-energy physics is effectively driven toward an over-screened Kondo-like regime, and the correct Fermi-liquid limit cannot be properly recovered [105–107]. At low temperatures, this deficiency leads to a non-monotonic convergence with the expansion order of the self-energy at low frequencies: The XCA self-energy can display an unphysical finite positive imaginary part at low positive frequencies, as shown in the inset of the left panel of Fig. 3.2. However, the convergence is smoother at higher frequencies, even though it does not attain the same level of accuracy as the reference solution. To the best of our knowledge, this work provides the first systematic exploration, up to fifth order in the strong-coupling expansion, of both frequency-dependent quantities and static observables in the metal-to-Mott-insulator transition of the single-band Hubbard model.

We conclude this subsection by discussing the timings for a single impurity solution within a DMFT iteration in Fig. 3.2. The MC reference solution requires on the order of a few hours, comparable to the cost of the fourth-order expansion. In the insulating regime, however, the third-order expansion already achieves an accuracy comparable to the MC result while being roughly three orders of magnitude faster, requiring only a few seconds. This difference in performance reflects the distinct scaling of the two methods

with inverse temperature β . The computational cost of CTHYB scales as β^3 [73], whereas the XCA method exploits the discrete Lehmann representation (DLR) [42, 43], whose basis size grows only logarithmically with β . As a result, the cost per diagram increases only mildly as the temperature is lowered. Consequently, the performance advantage of XCA over CTHYB is expected to become even more pronounced near and below the Mott critical point. We note, however, that the main bottleneck of the XCA method is the rapid increase in computational cost with expansion order, due to the factorial growth in the number of diagrams that must be evaluated [42, 43].

3.3.2 Static and thermodynamic quantities

We now move our attention to the static and thermodynamic quantities characterizing the metallic and insulating solutions in the half-filled system. These converge faster than the dynamical quantities, even in the metallic case, as they are less sensitive to the low-frequency Fermi-liquid behavior that is poorly described. In Fig. 3.3 we show the expectation value of the double occupancy $\langle n_{\uparrow}n_{\downarrow} \rangle$ and the total energy per site E_{site} across the metal to Mott insulator crossover ($\beta = 10$), critical point ($\beta = 18$), and first order transition ($\beta = 36$). The double occupancy is a measure of the local charge fluctuations, which are suppressed in the Mott insulating phase, while the energy per site is a thermodynamic quantity that also includes a contribution from the kinetic energy. Both quantities show a clear crossover from the metallic to the insulating behavior as U increases, with a more pronounced variation as the temperature is lowered towards the critical point. Below the critical temperature, the double occupancy and energy per site show a discontinuous jump at the first order transition, with a coexistence region where both metallic and insulating solutions can be stabilized. The XCA method is able to capture the overall trends of these quantities across the crossover, critical point, and first order transition, even in the metallic regime. However, the convergence with the expansion order is faster in the insulating regime, where the solution is adiabatically connected to the atomic limit. In the metallic regime, the low-order expansion overestimates the interaction effects, leading to a bias toward the insulating solution, while third order expansion already gives a good agreement with the reference solution.

In Fig. 3.4 we show the convergence of the energy per site with the expansion order for the metallic ($U = 3$) and insulating ($U = 5$) cases at $\beta = 36$. The energy per site converges faster than the dynamical quantities, e.g. the self-energy. Once again, in the insulating case, the third expansion order is already within the accuracy of the reference solution. In the metallic case, the convergence is slower than the insulating one, but the relative difference with respect to the reference solution is better as compared to the frequency dependent self-energy. It's also important to notice that the convergence on the potential and kinetic energy is approached with opposite bias, as we can see in Fig. 3.5, which compensates and leads to a more accurate total energy. This is not a coincidence: lower expansion orders are biased towards a more correlated solution,

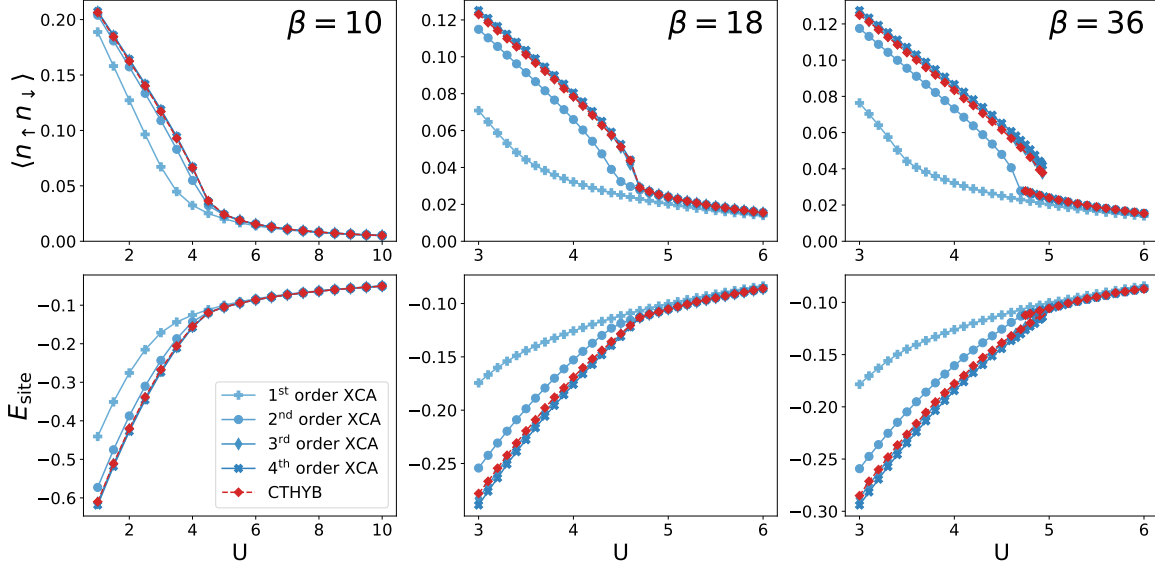


Figure 3.3: Double occupancy $\langle n_{\uparrow} n_{\downarrow} \rangle$ and total energy per site E_{site} across the metallic to Mott insulating crossover ($\beta = 10$), critical point ($\beta = 18$), and first order transition ($\beta = 36$). Third order expansion already gives a good agreement with the reference solution, even in the metallic regime. As expected, the convergence is faster in the insulating phase.

which has a lower potential energy and a higher kinetic energy.

Interestingly, the potential and kinetic energy show a non-monotonic behavior with the temperature in the metallic and insulating solution, respectively. The minimum in the potential energy of the metallic solution is a signature of the Pomeranchuk effect, which we will discuss in more detail in the next subsection; the minimum in the kinetic energy of the insulating solution is, on the other side, due to the gain in kinetic energy as particle-hole excitations are thermally activated in the Mott insulating phase, which is a signature of the crossover from a localized to a more itinerant regime at finite temperature. To corroborate this interpretation, in the insets of Fig. 3.5 we show the evolution of the minimum location as a function of the interaction strength U : the temperature minimum scales linearly with U and thus with the Mott gap, which is the relevant energy scale for the thermal activation of particle-hole excitations in the Mott insulating phase.

Entropy, Pomeranchuk effect and lattice free energy

A key advantage of the XCA algorithm is that it provides access to the impurity free energy, a quantity that is typically difficult to obtain with standard impurity solvers. From the latter, we can then compute the lattice free energy and entropy. In Fig. 3.6 we show the entropy as a function of temperature for different values of U , corresponding to the weakly correlated metal ($U = 2$), strongly correlated metal ($U = 4$), and Mott insulator ($U = 5$). While the entropy at a given temperature can be computed within a single calculation using the XCA solver, within MC solvers one needs to perform a

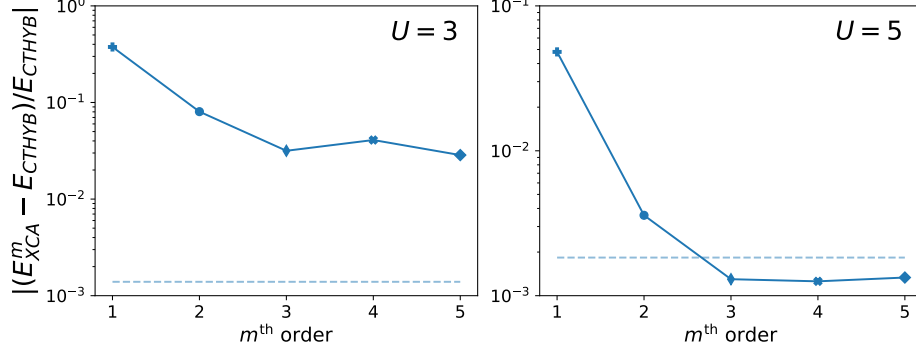


Figure 3.4: Relative difference of the energy per site with respect to the reference solution for a metallic ($U = 3$) and insulating ($U = 5$) solution at $\beta = 36$. The horizontal dashed lines indicate the estimated relative accuracy of the CTHYB reference solution, computed as the standard deviation over ten independent runs.

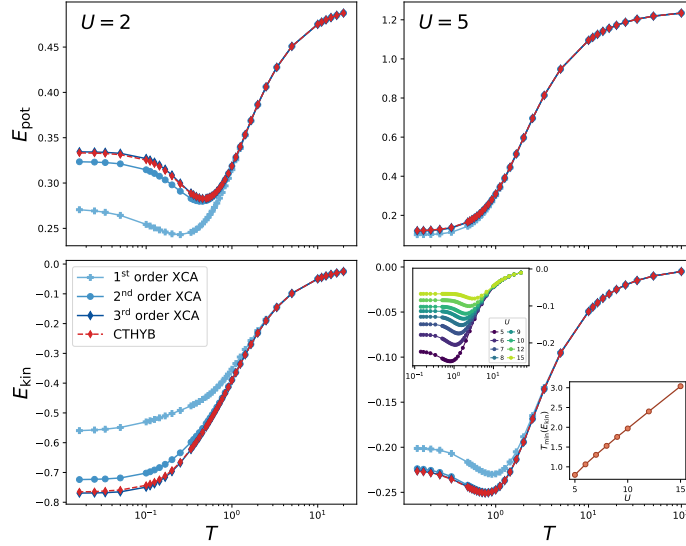


Figure 3.5: Potential and kinetic energy per site as a function of temperature for the metallic ($U = 2$) and insulating ($U = 5$) solutions. The insets show the evolution of the temperature location of the minimum as a function of the interaction strength U . The minimum in the potential energy of the metallic solution is a signature of the Pomeranchuk effect, while the minimum in the kinetic energy of the insulating solution is due to the gain in kinetic energy as particle-hole excitations are thermally activated in the Mott insulating phase.

thermodynamic integration of the energy per site, which requires multiple calculations at different temperatures. One starts from a reference point for which the entropy is known, e.g. the infinite temperature limit where $S = \ln(4)$ for the half-filled Hubbard model, and integrates the Maxwell relation $T\partial S/\partial T = \partial E/\partial T$ down to the desired temperature,

$$S(T) = S(T_{\text{ref}}) + \int_{T_{\text{ref}}}^T \frac{1}{T'} \frac{\partial E}{\partial T'} dT'. \quad (3.60)$$

To improve the numerical stability of the integration, it is better to perform the integration in the inverse temperature β instead of the temperature T , which leads to

$$S(\beta) = S(\beta_{\text{ref}}) + [\beta' E(\beta')]_{\beta_{\text{ref}}}^{\beta} - \int_{\beta_{\text{ref}}}^{\beta} E(\beta') d\beta'. \quad (3.61)$$

We stress that this procedure is not only computationally expensive, as it requires multiple calculations at different temperatures, but it is also prone to numerical errors, as it involves a numerical integration of the energy per site, which can be noisy due to the statistical error of the MC sampling. Moreover, the choice of the reference point and the integration path can also affect the final result. All these issues are circumvented in the XCA solver, where the entropy can be directly computed from a single calculation at the desired temperature.

In the metallic regime, the entropy decreases monotonically as we decrease the temperature, as expected for a Fermi liquid. However, our finite order expansion does not capture the correct low-temperature behavior of the metallic solution, and the entropy does not go to zero at zero temperature, as it should for a Fermi liquid. Looking at the insets of the left and middle upper panels of Fig. 3.6, we can see that the entropy at low temperature deviates from the linear in T behavior expected for a Fermi liquid, and it shows a finite intercept at zero temperature, which is a signature of the over-screened Kondo-like regime driven by the NCA approximation. Increasing the expansion order improves the accuracy of the entropy, and pushes the deviation from the Fermi liquid regime to lower temperatures. Differently, in the Mott insulating regime the entropy saturates at low temperature to a finite value $S = \ln(2)$, which is a signature of the localized magnetic moments of the non-magnetic solution. Surprisingly, the entropy in the Mott insulating regime is already very well reproduced at the first order expansion: we believe this is due to the fact that in the insulating regime the kinetic and potential energy contributions to the total energy are separately not very accurate at low expansion order, but their biases compensate leading to a more accurate total energy and entropy per site already at low expansion order.

An interesting entropic effect captured by the DMFT metallic solution of the Hubbard model is the Pomeranchuk effect, which is associated with a non-monotonic temperature dependence of the double occupancy, as shown in Fig. 3.6. Naively we would expect that the double occupancy increases monotonically with temperature, as thermal fluctuations enhance local charge fluctuations. However, in the correlated metallic regime, the double occupancy initially decreases upon increasing the temperature from zero, before eventually increasing at higher temperatures. This counterintuitive behavior

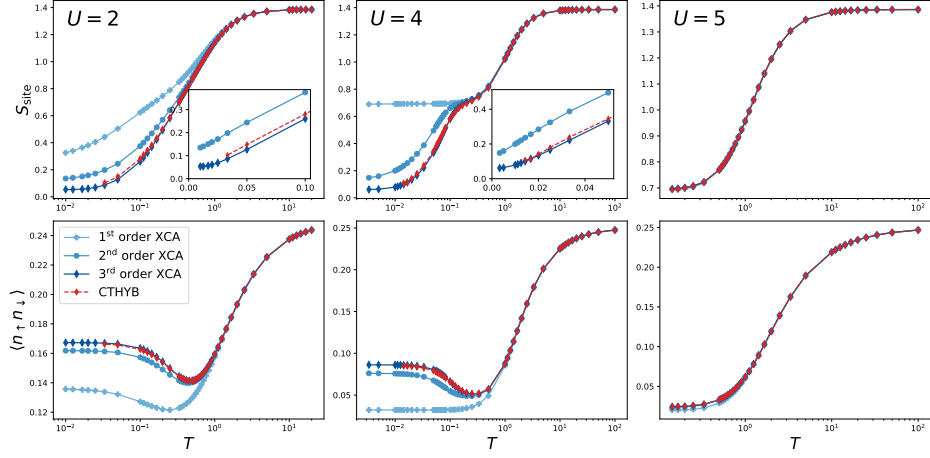


Figure 3.6: First row: Entropy as a function of temperature for different values of U , corresponding to the weakly correlated metal ($U = 2$), strongly correlated metal ($U = 4$), and MI ($U = 5$). In the insets, we show that the entropy at low temperature deviates from the linear in T behavior expected for a Fermi liquid, and it shows a finite intercept at zero temperature. Increasing the expansion order pushes the deviation from the Fermi liquid regime to lower temperatures. In the Mott insulating regime, the entropy correctly saturates at low temperature to a finite value $S = \ln(2)$, which is a signature of the localized magnetic moments of the non-magnetic solution.

Second row: Double occupancy as a function of temperature for the same values of U . In the metallic regime, the double occupancy clearly shows the Pomeranchuk effect. The minimum location shifts to lower temperatures increasing the interaction strength, as the Kondo temperature decreases approaching the Mott transition.

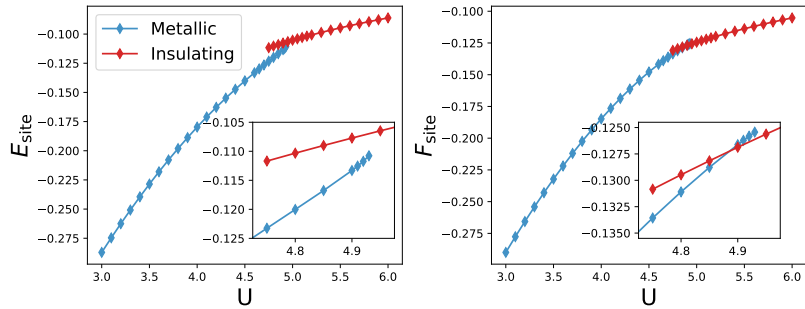


Figure 3.7: Total energy and free energy per site across the first-order transition at $\beta = 36$. Although the metallic solution has a lower energy than the insulating one throughout the coexistence region, their free energies cross at $U \approx 4.9$, thereby identifying the location of the first-order transition.

is a manifestation of the Pomeranchuk effect, which arises from the entropic stabilization of local moments at finite temperature. In other words, as the temperature increases, the system favors a more localized state with lower double occupancy, due to the higher entropy associated with local moment formation. The Pomeranchuk effect is correctly reproduced by our XCA solver at any expansion order, but the accuracy on the double-occupancy minimum location improves increasing the expansion order and third order already gives a very good agreement with the reference solution. As expected, the minimum shifts to lower temperatures increasing the interaction strength, as the Kondo temperature decreases approaching the Mott transition. In the Mott insulating regime, the double occupancy is very small at low temperature, and it does not show the Pomeranchuk effect, as the system is already in a localized regime at low temperature.

Finally, we conclude this subsection by looking at the energy and free energy per site across the first order transition with $\beta = 36$, as shown in Fig. 3.7. By seeding the DMFT loop with the metallic or insulating solutions, we can stabilize both solutions in the coexistence region. Across all the coexistence region the energy per site of the metallic solution is always lower than the insulating one. By considering only the energy per site, one would naively conclude that the metallic solution is always thermodynamically favored. However, the relevant thermodynamic potential is the free energy, whose minimization determines the location of the first-order transition. Since at low temperature the metallic solution possesses a lower entropy than the insulating one, it is natural to expect that, within part of the coexistence region, the insulating phase may acquire a lower free energy despite its higher internal energy. In this regime, the system is therefore expected to be insulating even though a metastable metallic solution can still be stabilized. This scenario is indeed confirmed in Fig. 3.7, where the free energies of the metallic and insulating solutions cross at $U \approx 4.9$, thereby identifying the location of the first-order transition. These results were obtained using the third-order expansion, which accurately reproduces the behavior of the relevant observables across the transition, in agreement with the reference solution discussed in Fig. 3.3. This analysis underscores the importance of accessing the free energy in order to accurately determine the location of finite temperature thermodynamic transitions.

3.3.3 Away from half-filling

The validity of the analysis presented in the previous subsections is not limited to the half-filled system, but it can be extended to the doped case as well. In this subsection, we explicitly show it on the example of the Mott insulating solutions at $U = 5$ and $\beta = 18$, which we dope with electrons by changing the chemical potential $\mu = U/2 + \delta\mu$, with $\delta\mu > 0$.

In Fig. 3.8 we show the Matsubara Green's function and self-energy for a value of the chemical potential corresponding to an electron doping of approximately 10% with

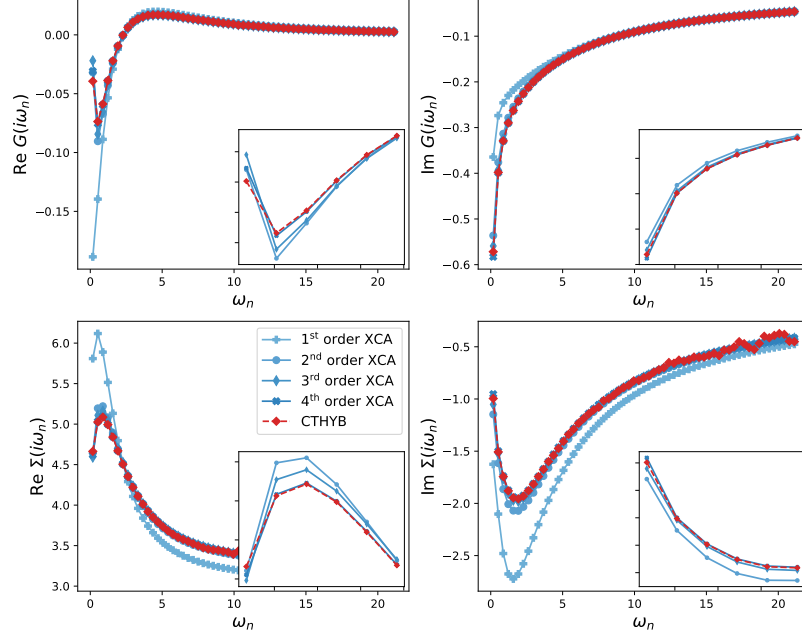


Figure 3.8: Matsubara Green's function $G(i\omega_n)$ and self-energy $\Sigma(i\omega_n)$ for the doped Mott insulator at $U = 5$ and $\beta = 18$, for a value of the chemical potential corresponding to an electron doping of approximately 10% with respect to half-filling ($\delta\mu = 1.6$). Both imaginary and real parts are shown, as the real part is no longer zero by particle-hole symmetry. The insets zoom on the low-frequency regime (first 6 positive Matsubara frequencies).

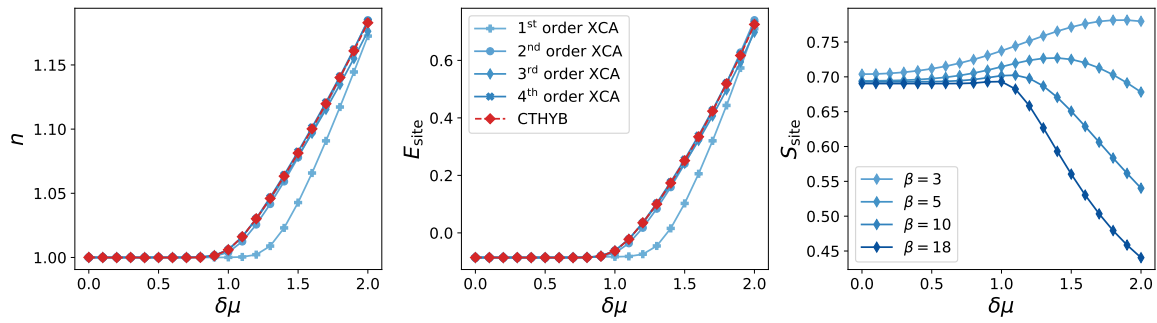


Figure 3.9: In the first two panels we show the occupation number and total energy per site as functions of the chemical-potential deviation from half-filling for a doped Mott insulator at $U = 5$ and $\beta = 18$. The plateau around half-filling is a signature of the Mott gap, which is overestimated at low expansion order.

In the third panel we show the entropy, computed at the third-order expansion, for different values of the temperature. It presents a local maximum in the lightly doped regime, reflecting the competition between localized and itinerant electronic behavior.

respect to half-filling. Both imaginary and real part are shown, as the real part is no longer zero by particle-hole symmetry ($\delta\mu = 1.6$). In the metallic regime at low temperature, we observe the same limitations discussed for the undoped case, e.g. a non-monotonic convergence of the self-energy and Green's function, particularly at low frequencies.

Moving to static observables, in Fig. 3.9 we show the occupation number and total energy per site as a function of the chemical potential deviation from half-filling. Both quantities show a plateau around half-filling, which is a signature of the Mott gap. The first order expansion overestimates the interaction effects, and, consequently, the plateau size in the Mott gap.

An intriguing aspect of the doped Mott insulator, which is readily accessible with the XCA solver, is the behavior of the entropy across the doping-driven Mott transition. In Fig. 3.9, we show the entropy as a function of the chemical potential deviation from half-filling. In the insulating solution, the entropy remains close to its half-filled value until the Hubbard bands begin to be doped. At that point, it increases as charge fluctuations become more pronounced. This reflects the larger number of accessible states in the lightly doped Mott insulator owing to the presence of mobile charge carriers. Upon further doping, however, the system crosses over toward a more metallic regime, where the entropy decreases again as electronic coherence is progressively restored and localization effects are reduced. The resulting local maximum of the entropy in the lightly doped regime reflects the competition between localized and itinerant electronic behavior, and is a clear manifestation of strong electronic correlations. This effect becomes progressively less pronounced as the temperature is lowered, consistent with the enhanced coherence of the low-temperature metallic state.

A delicate aspect of the doped case concerns the determination of the high-frequency limit of the real part of the self-energy, namely the Hartree shift,

$$\Sigma_H \equiv \text{Re } \Sigma_\sigma(i\omega_n \rightarrow \infty) = U \langle n_{\bar{\sigma}} \rangle. \quad (3.62)$$

At half-filling, particle-hole symmetry enforces the correct value of the Hartree shift to $U/2$, independently of the expansion order. Away from half-filling, however, this is no longer the case, and Σ_H must be determined with care. This quantity is required, for instance, to correctly embed the DMFT self-energy in a Density Functional Theory (DFT)+DMFT calculation through the double-counting correction, or to represent the self-energy in the DLR basis, where the correct high-frequency limit must be supplied as input.

There are two natural ways to determine Σ_H . The first is the operator estimator, which evaluates the Hartree term directly as

$$\Sigma_H = U \langle n_{\bar{\sigma}} \rangle. \quad (3.63)$$

The second is a tail fit: since

$$\text{Re } \Sigma(i\omega_n) \rightarrow \Sigma_H + \mathcal{O}(\omega_n^{-2}) \quad (3.64)$$

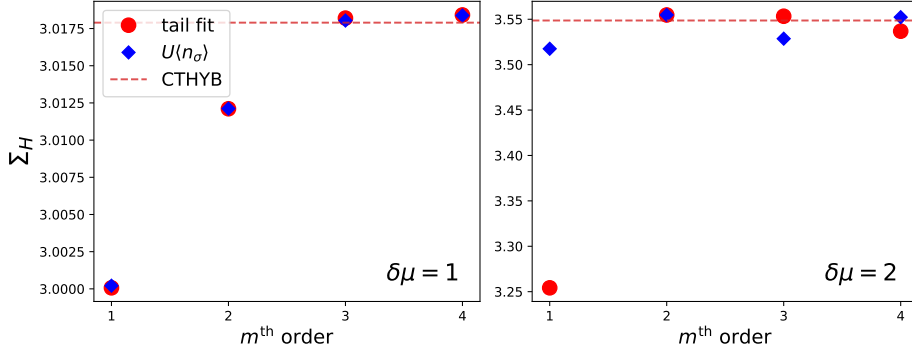


Figure 3.10: Hartree shift $\Sigma_H = \text{Re} \Sigma(i\omega_n \rightarrow \infty)$ for the doped Mott insulator at $U = 5$ and $\beta = 18$, shown as a function of the expansion order. Two estimates are compared: the operator estimator, $\Sigma_H = U\langle n_{\bar{\sigma}} \rangle$, and the value obtained from a tail fit of $\text{Re} \Sigma(i\omega_n)$. The horizontal dashed line indicates the CTHYB reference result. The tail-fit estimate follows the actual high-frequency limit of the approximate XCA self-energy and can differ from $U\langle n_{\bar{\sigma}} \rangle$ at finite expansion order.

at large frequencies, Σ_H can be extracted by fitting the asymptotic behavior of the computed self-energy. In an exact solver, the two procedures must agree. In an approximate solver, however, they need not coincide, and their discrepancy provides a direct measure of the systematic error introduced by truncating the diagrammatic expansion.

Because the XCA self-energy is entirely free of stochastic noise, the tail-fit estimate can be performed with high precision. Nevertheless, a clear discrepancy between the two estimates is visible in Fig. 3.10: at finite expansion order, the tail-fit value of Σ_H does not coincide with $U\langle n_{\bar{\sigma}} \rangle$, and the mismatch decreases but does not vanish as the order is increased. This behavior reflects the fact that a truncated skeleton expansion does not exactly satisfy the high-frequency sum rules of the interacting Green’s function.

The operator estimator $U\langle n_{\bar{\sigma}} \rangle$ converges more rapidly to the correct physical value, and is therefore preferable when the Hartree shift is needed as a standalone observable. By contrast, when the goal is to use the XCA self-energy in an internally consistent way — for example, to represent it in the DLR basis or to extract the double-counting correction in a DFT+DMFT calculation — the tail-fit estimate should be used, because it reflects the actual high-frequency behavior of the approximate $\Sigma(i\omega_n)$. The two estimates are therefore complementary: the operator estimator provides the converged physical Hartree shift, whereas the tail fit provides the Hartree shift that is consistent with the approximate self-energy itself.

3.4 Conclusions

We have discussed how a pseudoparticle representation of the many-body states of a quantum impurity problem underlies a deterministic, strong-coupling solver for dy-

namical mean-field theory. Beyond the dynamical single-particle Green's function, the solver provides direct access to static and thermodynamic quantities, most notably the impurity free energy.

We have benchmarked the solver on the single-band Hubbard model on a Bethe lattice, across the metal-to-Mott-insulator transition and down to low temperatures. Convergence with the expansion order is fast in the insulating phase, which is adiabatically connected to the atomic limit, where the third order already matches the continuous-time Monte Carlo reference within its statistical accuracy while being orders of magnitude computationally cheaper. However, in the metallic phase the convergence is slower, and the low-order truncation inherits the over-screened low-energy behavior of the non-crossing approximation, so that the correct Fermi-liquid limit is recovered only gradually, and not monotonically, as the order is increased. Nevertheless, static and thermodynamic observables converge substantially faster than dynamical quantities. The solver accurately reproduces the double occupancy, energy per site, and entropy. It captures both the residual entropy $S = \ln 2$ of the paramagnetic Mott insulator within DMFT and the Pomeranchuk effect in the correlated metal. Most importantly, the explicit free energy balance identifies which of the coexisting metallic and insulating solutions is thermodynamically stable. It thus locates the first-order transition line directly, without relying on an indirect reconstruction of the thermodynamic potential. The same framework applies naturally away from half-filling.

The deterministic and noise-free character of the method, its immunity to the sign problem, and its direct access to thermodynamic potentials make it a valuable complement to the stochastic solvers that currently dominate the field. These advantages become particularly significant at low temperatures, where the use of a discrete Lehmann representation leads to a computational cost that increases only mildly with inverse temperature [42, 43]. The limitations are equally clear: The factorial growth of the number of diagrams with the expansion order currently restricts systematic convergence in the metallic Fermi-liquid regime, while low-order truncations retain an intrinsic bias toward the atomic limit.

This XCA solver holds promising potential in regimes where stochastic methods become prohibitively expensive. This occurs, for example, in multiorbital and spin-orbit coupled models, where the sign problem severely restricts the accessible temperature range. By extending controlled calculations into these regimes, more efficient impurity solvers broaden the range of correlated systems that can be investigated. Their underlying physical mechanisms can then be analyzed through the effective one-body descriptions that form the common thread of this thesis.

CHAPTER 4

Topology, correlations and magnetism with the ghost-Gutzwiller Ansatz

In this chapter, we discuss how the ghost-Gutzwiller framework provides an interpretable band-structure picture for correlated topological phases, capturing non-perturbative effects. Most notably, we reveal the emergence of topologically nontrivial Hubbard bands hosting their own edge states, and the possibility of tuning their topology through a finite magnetization. This chapter is based on Ref. [44].

Introduction

Among the key guiding principles in modern condensed matter physics, band-structure topology and strong electronic correlations have emerged as central paradigms for understanding and designing materials with tailored conducting and magnetic properties. Band topology provides a robust classification of gapped phases of noninteracting electrons in terms of global properties of their Bloch wavefunctions, and predicts protected boundary modes that are robust to disorder and to a wide class of perturbations [69, 70]. Strong electronic correlations underlie the most striking phenomena observed in quantum materials, from high-temperature superconductivity [19] to the Mott metal–insulator transition [26, 108]. Furthermore, strongly correlated phases of matter are arguably characterized by their tunability, i.e., the fact that slight modifications of external parameters like pressure, physical or chemical doping, or temperature result in dramatic changes of the electronic structure [109, 110]. The combination of these two paradigms is then a natural place to look for new quantum phases of matter, and recent experimental landmarks—from chiral Kondo lattices [111] to fractional quantum anomalous Hall states in moiré transition-metal dichalcogenides [112, 113]—confirm that it is currently driving the field.

Understanding their interplay remains a central challenge in condensed matter physics, primarily hindered by a language mismatch problem. While band topology is naturally formulated within single-particle band theory, with topological invariants defined as global properties of the Bloch Hamiltonian or of the noninteracting one-body Green’s function [53, 63], strong correlations typically elude such an effective one-body descrip-

tion. In weakly correlated systems, effective single-particle descriptions such as density functional theory (DFT) [7, 8, 114] can offer invaluable insights for guiding material design [115–119], but fall short when interaction effects dominate over the band energy gain. Conversely, state-of-the-art methods for strongly correlated systems, such as dynamical mean-field theory (DMFT) [26, 120, 121], excel at describing local correlation effects across the full bandwidth, but are not naturally formulated around a band-structure picture applicable at both low- and high-energy scales, which is the most direct language to address interband coherence effects relevant to topology. The aim of this chapter is to show that the ghost-Gutzwiller (gGut) variational embedding framework [122–125], which has attracted growing interest in recent years [126–136], offers a particularly transparent way to bridge this gap. By enlarging the variational Hilbert space of the uncorrelated reference state with auxiliary, “ghost”, orbitals, the gGut method delivers an effective quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$ that encodes, in a band-structure language, both the low-energy coherent quasiparticles and the high-energy Hubbard-band features. Thus the entire toolbox developed for noninteracting topological band theory (band resolved Chern numbers, symmetry-based indicators, ...) can then be readily applied to $H_{\text{qp}}(\mathbf{k})$. This approach enables an interpretable and computationally efficient treatment of correlated topological phases, resulting in energy- and momentum-resolved topological features that are directly comparable to experimental spectra. We exemplify the advantages of this framework through a detailed study of the interacting Bernevig-Hughes-Zhang (BHZ) model [31].

The chapter is organized as follows. In Sec. 4.1 we review the key ingredients of the ghost-Gutzwiller formalism, introducing the variational objects, the Gutzwiller constraints, and the effective quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$ that lies at the heart of our approach. In Sec. 4.2 we show how band-structure topology can be addressed within this framework: after establishing a spectral representation of the correlated electrons in terms of the gGut Green’s function (Sec. 4.2.1), we demonstrate that the Chern numbers of the quasiparticle bands of $H_{\text{qp}}(\mathbf{k})$ are physically meaningful and directly related to the topological invariant of the fully interacting system. In Sec. 4.3 we benchmark the method on the interacting BHZ model and develop the quasiparticle perspective on the correlated topological transition. In Sec. 4.4 we turn to open boundary conditions, showing that the topological edge states are directly encoded in the quasiparticle Hamiltonian, and we investigate how correlations themselves are reshaped at the boundaries, uncovering a nontrivial interplay between topology, interactions and finite-size effects. In Sec. 4.5 we present our most striking result, namely the emergence of topologically nontrivial Hubbard bands hosting their own edge states, and we analyze the interplay between topology, magnetism and correlation, showing that the topology of the Hubbard bands can be tuned through a finite magnetization.

4.1 Overview of the ghost-Gutzwiller formalism

In this section we review the key ingredients of the ghost-Gutzwiller formalism: The goal is not to present the full derivation of the method, which can be found in detail in the literature [122, 137–141], but to introduce the variational objects, the constraints, and the effective quasiparticle description that make the method so powerful for studying correlated topological phases. This discussion will also set the notation for the extension to non-local interactions presented in the next chapter.

For the purposes of this chapter, we consider a generic multi-orbital Hubbard Hamiltonian

$$H = - \sum_{\mathbf{R}\mathbf{R}'} \sum_{\alpha\beta} t_{\mathbf{R}\mathbf{R}'}^{\alpha\beta} c_{\mathbf{R}\alpha}^\dagger c_{\mathbf{R}'\beta} + \sum_{\mathbf{R}} H_{\text{loc}}(\mathbf{R}), \quad (4.1)$$

where $c_{\mathbf{R}\alpha}^\dagger$ creates an electron in the state α at site $\mathbf{R}$, $\alpha, \beta = 1, \dots, N_{\text{phys}}$ include both orbital and spin degrees of freedom, $t_{\mathbf{R}\mathbf{R}'}^{\alpha\beta}$ are the inter-site hopping amplitudes, and $H_{\text{loc}}(\mathbf{R})$ contains all local one-body and two-body terms.

The gGut wavefunction is defined as

$$|\Psi_{\text{gGut}}\rangle = \mathcal{P} |\psi_{\text{qp}}\rangle = \prod_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} |\psi_{\text{qp}}\rangle, \quad (4.2)$$

with $|\psi_{\text{qp}}\rangle$ an uncorrelated quasiparticle wavefunction, a Slater determinant or BCS state, defined in an auxiliary Hilbert space with $N_{\text{aux}} \geq N_{\text{phys}}$ orbitals per site. The gGut Ansatz extends the conventional Gutzwiller wavefunction by introducing auxiliary "ghost" degrees of freedom, enlarging the variational Hilbert space of the uncorrelated state $|\psi_{\text{qp}}\rangle$. This, in turn, enables the gGut wavefunction to describe the physics of both low-energy coherent quasiparticles and high-energy spectral features, such as the Hubbard bands.

The local operator $\mathcal{P}_{\mathbf{R}}$ is a projector from the auxiliary quasiparticle local Hilbert space to the physical one:

$$\mathcal{P}_{\mathbf{R}} = \sum_{\Gamma n} \lambda_{\Gamma n}(\mathbf{R}) |\Gamma, \mathbf{R}\rangle \langle n, \mathbf{R}|, \quad (4.3)$$

where $|n, \mathbf{R}\rangle$ and $|\Gamma, \mathbf{R}\rangle$ span, respectively, the physical and auxiliary local Hilbert spaces.

The analytical evaluation of expectation values on the gGut wavefunction becomes possible in the infinite-coordination limit once the following Gutzwiller constraints are imposed:

$$\begin{aligned} \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger \mathcal{P}_{\mathbf{R}} | \psi_{\text{qp}} \rangle &= 1, \\ \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger \mathcal{P}_{\mathbf{R}} f_{\mathbf{R}a}^\dagger f_{\mathbf{R}b} | \psi_{\text{qp}} \rangle &= \langle \psi_{\text{qp}} | f_{\mathbf{R}a}^\dagger f_{\mathbf{R}b} | \psi_{\text{qp}} \rangle \equiv \Delta_{ab}(\mathbf{R}), \end{aligned} \quad (4.4)$$

with $f_{\mathbf{R}a}^\dagger$ and $f_{\mathbf{R}b}$ creation and annihilation operators of the auxiliary quasiparticles, and $\Delta_{ab}(\mathbf{R})$ their local single-particle density matrix in the quasiparticle state. The first constraint fixes the normalization of the projected wavefunction, while the second ensures that the local auxiliary density matrix is unchanged by the action of the projector.

It is useful to absorb the local probability distribution of the uncorrelated state into a positive semi-definite matrix $\hat{P}_0(\mathbf{R})$

$$(\hat{P}_0(\mathbf{R}))_{nm} \equiv \langle \psi_{\text{qp}} | m, \mathbf{R} \rangle \langle n, \mathbf{R} | \psi_{\text{qp}} \rangle, \quad (4.5)$$

and introduce $\hat{\Phi}(\mathbf{R})$ through

$$\hat{\lambda}(\mathbf{R}) = \hat{\Phi}(\mathbf{R}) \sqrt{\hat{P}_0(\mathbf{R})^{-1}}. \quad (4.6)$$

With this parametrization, the Gutzwiller constraints take the compact form

$$\begin{aligned} \text{Tr}(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\Phi}(\mathbf{R})) &= 1, \\ \text{Tr}(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\Phi}(\mathbf{R}) \hat{f}_{\mathbf{R}a}^\dagger \hat{f}_{\mathbf{R}b}) &= \Delta_{ab}(\mathbf{R}). \end{aligned} \quad (4.7)$$

The hats on the fermionic operators indicate their matrix representation in the local auxiliary Fock basis. The advantage of the $\hat{\Phi}(\mathbf{R})$ parametrization is that local expectation values, constraints, and eventually the embedding construction all take a trace form that is independent of the explicit probabilities contained in $\hat{P}_0(\mathbf{R})$.

4.1.1 Computing expectation values of local and non-local operators

As we anticipated to motivate the introduction of the Gutzwiller constraints (4.4), a key strength of the gGut formalism is that expectation values of both local and non-local operators can be evaluated analytically on the wavefunction (4.2) once the infinite-coordination limit is taken. The identities discussed below are therefore exact in this limit; when used for finite-coordination lattices, they define the *Gutzwiller approximation* (GA).

Let us then discuss the relevant identities propedeutic to the evaluation of the ground state energy or any other relevant physical operator. We start considering the expectation value of a generic local operator $\mathcal{O}_{\mathbf{R}}$ composed of an even number of fermionic operators:

$$\begin{aligned} \langle \Psi_{\text{gGut}} | \mathcal{O}_{\mathbf{R}} | \Psi_{\text{gGut}} \rangle &= \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger \mathcal{O}_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} | \psi_{\text{qp}} \rangle \\ &= \text{Tr}(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\mathcal{O}}_{\mathbf{R}} \hat{\Phi}(\mathbf{R})). \end{aligned} \quad (4.8)$$

Similarly for non-local operators $\mathcal{O}_{\mathbf{R}\mathbf{R}'}$ acting on the two sites $\mathbf{R}$ and $\mathbf{R}'$,

$$\langle \Psi_{\text{gGut}} | \mathcal{O}_{\mathbf{R}\mathbf{R}'} | \Psi_{\text{gGut}} \rangle = \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger \mathcal{P}_{\mathbf{R}'}^\dagger \mathcal{O}_{\mathbf{R}\mathbf{R}'} \mathcal{P}_{\mathbf{R}} \mathcal{P}_{\mathbf{R}'} | \psi_{\text{qp}} \rangle. \quad (4.9)$$

In the Hamiltonian Eq. (4.1), the non-local contributions are the hopping processes $c_{\mathbf{R}\alpha}^\dagger c_{\mathbf{R}'\beta}$, whose expectation value is given by

$$\begin{aligned} \langle \Psi_{\text{gGut}} | c_{\mathbf{R}\alpha}^\dagger c_{\mathbf{R}'\beta} | \Psi_{\text{gGut}} \rangle &= \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger c_{\mathbf{R}\alpha}^\dagger \mathcal{P}_{\mathbf{R}} \mathcal{P}_{\mathbf{R}'}^\dagger c_{\mathbf{R}'\beta} \mathcal{P}_{\mathbf{R}'} | \psi_{\text{qp}} \rangle \\ &= \sum_{ab=1}^{N_{\text{aux}}} \mathcal{R}_{a\alpha}^\dagger(\mathbf{R}) \mathcal{R}_{\beta b}(\mathbf{R}') \langle \psi_{\text{qp}} | f_{\mathbf{R}a}^\dagger f_{\mathbf{R}'b} | \psi_{\text{qp}} \rangle, \end{aligned} \quad (4.10)$$

where $\hat{\mathcal{R}}(\mathbf{R})$ is a rectangular wave-function renormalization matrix, with N_{phys} rows and N_{aux} columns. This matrix encodes how the on-site projector redistributes the physical electron spectral weight among the auxiliary quasiparticle degrees of freedom. Equivalently, within inter-site single-particle expectation values, the projected physical operators are replaced by renormalized auxiliary operators:

$$\mathcal{P}_{\mathbf{R}}^\dagger c_{\mathbf{R}\alpha} \mathcal{P}_{\mathbf{R}} \rightarrow \sum_{a=1}^{N_{\text{aux}}} \mathcal{R}_{\alpha a}(\mathbf{R}) f_{\mathbf{R}a}. \quad (4.11)$$

This identification should be understood only at the level of inter-site single-particle expectation values, and not as an operator identity in the full local Hilbert space. The renormalization matrices $\hat{\mathcal{R}}(\mathbf{R})$ are determined by the algebraic equation

$$\langle \psi_{\text{qp}} | f_{\mathbf{R}a}^\dagger \mathcal{P}_{\mathbf{R}}^\dagger c_{\mathbf{R}\beta} \mathcal{P}_{\mathbf{R}} | \psi_{\text{qp}} \rangle = \sum_{b=1}^{N_{\text{aux}}} \mathcal{R}_{\beta b}(\mathbf{R}) \Delta_{ab}(\mathbf{R}). \quad (4.12)$$

Combining the local contribution from H_{loc} with the renormalized hopping expectation value, we obtain the variational gGut energy for the multi-orbital Hubbard model of Eq. 4.1:

$$E[\{\hat{\Phi}(\mathbf{R})\}_{\mathbf{R}}, |\psi_{\text{qp}}\rangle] = \langle \psi_{\text{qp}} | \tilde{H}_{\text{qp}} | \psi_{\text{qp}} \rangle + \sum_{\mathbf{R}} \text{Tr} \left(\hat{\Phi}^\dagger(\mathbf{R}) \hat{H}_{\text{loc}}(\mathbf{R}) \hat{\Phi}(\mathbf{R}) \right), \quad (4.13)$$

where $\tilde{H}_{\text{qp}}$ is given by

$$\tilde{H}_{\text{qp}} = - \sum_{\mathbf{R}\mathbf{R}'} \sum_{ab=1}^{N_{\text{aux}}} \left(\sum_{\alpha\beta=1}^{N_{\text{phys}}} \mathcal{R}_{a\alpha}^\dagger(\mathbf{R}) t_{\mathbf{R}\mathbf{R}'}^{\alpha\beta} \mathcal{R}_{\beta b}(\mathbf{R}') \right) f_{\mathbf{R}a}^\dagger f_{\mathbf{R}'b}. \quad (4.14)$$

Thus, the effect of correlations on the kinetic part is encoded in the dressed hopping amplitudes $\hat{\mathcal{R}}^\dagger(\mathbf{R}) \hat{t}_{\mathbf{R}\mathbf{R}'} \hat{\mathcal{R}}(\mathbf{R}')$ of the auxiliary quasiparticles. The gGut ground-state wavefunction is obtained by minimizing $E[\{\hat{\Phi}(\mathbf{R})\}_{\mathbf{R}}, |\psi_{\text{qp}}\rangle]$ with respect to the variational parameters $\{\hat{\Phi}(\mathbf{R})\}_{\mathbf{R}}$ and $|\psi_{\text{qp}}\rangle$, under the Gutzwiller constraints. In practice, this constrained optimization is most conveniently reformulated as an embedding problem, in which the amplitudes $\hat{\Phi}(\mathbf{R})$ are encoded in an effective impurity wavefunction. This mapping is discussed in the next subsection.

4.1.2 Mapping to the impurity wavefunction

A generic Fock state in the auxiliary local Hilbert space is written as

$$|n, \mathbf{R}\rangle = \prod_{a=1}^{N_{\text{aux}}} (f_{\mathbf{R}a}^\dagger)^{n_a} |0\rangle, \quad n \equiv \{n_a\}, \quad (4.15)$$

with $n_a = 0, 1$. This state contains $n_{\text{qp}} = \sum_a n_a$ auxiliary particles. We now introduce, for each lattice site $\mathbf{R}$, an impurity wavefunction describing an impurity site coupled to

a discretized bath. The impurity degrees of freedom are labelled by $\alpha = 1, \dots, N_{\text{phys}}$, so that the impurity Fock space coincides with the physical local Hilbert space spanned by the states $|\Gamma\rangle$. The bath degrees of freedom are labelled by $a = 1, \dots, N_{\text{aux}}$ and are related to the auxiliary local Hilbert space by a particle-hole transformation. Given the auxiliary configuration $|n, \mathbf{R}\rangle$, the corresponding bath state is defined as

$$|\bar{n}\rangle \equiv \prod_{a=1}^{N_{\text{aux}}} (-1)^{(a-1)n_a} (f_a^\dagger)^{1-n_a} |0\rangle. \quad (4.16)$$

It contains $N_{\text{aux}} - n_{\text{qp}}$ bath particles. The phase convention in the definition of $|\bar{n}\rangle$ fixes the fermionic signs associated with the particle-hole transformation and allows the trace identities below to be written without additional sign factors. The embedded impurity wavefunction is then defined as

$$|\psi_{\text{imp}}(\mathbf{R})\rangle = \sum_{\Gamma n} \Phi_{\Gamma n}(\mathbf{R}) e^{i\phi_\Gamma} |\Gamma\rangle |\bar{n}\rangle, \quad (4.17)$$

where $\phi_\Gamma = \pi n_\Gamma(1 - n_\Gamma)/2$, and n_Γ is the number of physical electrons in the state $|\Gamma\rangle$. In this way, the variational parameters $\Phi_{\Gamma n}(\mathbf{R})$ are interpreted as the amplitudes of a many-body state in the enlarged impurity-bath Hilbert space. This mapping is useful because the traces involving $\hat{\Phi}(\mathbf{R})$ can be rewritten as expectation values over $|\psi_{\text{imp}}(\mathbf{R})\rangle$. Specifically, the Gutzwiller constraints take the form

$$\begin{aligned} \text{Tr}\left(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\Phi}(\mathbf{R})\right) &= \langle\psi_{\text{imp}}(\mathbf{R})|\psi_{\text{imp}}(\mathbf{R})\rangle = 1, \\ \langle\psi_{\text{qp}}|f_{\mathbf{R}a}^\dagger f_{\mathbf{R}b}|\psi_{\text{qp}}\rangle &= \langle\psi_{\text{imp}}(\mathbf{R})|f_b f_a^\dagger|\psi_{\text{imp}}(\mathbf{R})\rangle. \end{aligned} \quad (4.18)$$

The expectation value of a local operator $\hat{\mathcal{O}}_{\mathbf{R}}$ becomes

$$\text{Tr}\left(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\mathcal{O}}_{\mathbf{R}} \hat{\Phi}(\mathbf{R})\right) = \langle\psi_{\text{imp}}(\mathbf{R})|\mathcal{O}_{\mathbf{R}}|\psi_{\text{imp}}(\mathbf{R})\rangle. \quad (4.19)$$

In particular, this identity applies to the local Hamiltonian $H_{\text{loc}}(\mathbf{R})$. The remaining ingredient, necessary for computing the renormalized kinetic energy contribution, is the hybridization between the physical impurity and the bath degrees of freedom. If we define

$$\mathcal{Q}_{\beta a}(\mathbf{R}) \equiv \langle\psi_{\text{imp}}(\mathbf{R})|f_a^\dagger c_\beta|\psi_{\text{imp}}(\mathbf{R})\rangle = \text{Tr}\left(\hat{f}_{\mathbf{R}a}^\dagger \hat{\Phi}^\dagger(\mathbf{R}) \hat{c}_{\mathbf{R}\beta} \hat{\Phi}(\mathbf{R})\right), \quad (4.20)$$

together with the local quasiparticle density matrix $\hat{\Delta}(\mathbf{R})$, this determines the wavefunction renormalization matrix

$$\hat{\mathcal{R}}^\dagger(\mathbf{R}) = \left(\sqrt{\hat{\Delta}(\mathbf{R})^{-1}(\mathbb{I} - \hat{\Delta}(\mathbf{R}))^{-1}} \right)^T \hat{\mathcal{Q}}(\mathbf{R})^\dagger. \quad (4.21)$$

In terms of the embedded wavefunctions, the gGut variational problem can therefore be expressed as the saddle point of the Lagrange functional

$$\begin{aligned}
 \mathcal{L}[\{|\psi_{\text{imp}}(\mathbf{R})\rangle\}_{\mathbf{R}}, |\psi_{\text{qp}}\rangle, \{\mu_{ab}(\mathbf{R})\}_{\mathbf{R}}, \{\Lambda(\mathbf{R})\}_{\mathbf{R}}, \Lambda_{\text{qp}}] \\
 = \sum_{\mathbf{R}} \langle \psi_{\text{imp}}(\mathbf{R}) | H_{\text{loc}}(\mathbf{R}) | \psi_{\text{imp}}(\mathbf{R}) \rangle + \langle \psi_{\text{qp}} | \tilde{H}_{\text{qp}} | \psi_{\text{qp}} \rangle \\
 - \sum_{\mathbf{R}} \Lambda(\mathbf{R}) (\langle \psi_{\text{imp}}(\mathbf{R}) | \psi_{\text{imp}}(\mathbf{R}) \rangle - 1) - \Lambda_{\text{qp}} (\langle \psi_{\text{qp}} | \psi_{\text{qp}} \rangle - 1) \\
 - \sum_{\mathbf{R}} \sum_{ab=1}^{N_{\text{aux}}} \mu_{ab}(\mathbf{R}) \left[\langle \psi_{\text{imp}}(\mathbf{R}) | f_b^\dagger f_a | \psi_{\text{imp}}(\mathbf{R}) \rangle - \langle \psi_{\text{qp}} | f_{\mathbf{R}a}^\dagger f_{\mathbf{R}b} | \psi_{\text{qp}} \rangle \right].
 \end{aligned} \tag{4.22}$$

The multipliers $\Lambda(\mathbf{R})$ and Λ_{qp} enforce the normalization of the impurity and quasi-particle wavefunctions, respectively, while $\mu_{ab}(\mathbf{R})$ enforces the consistency between the bath density matrix and the local density matrix of the auxiliary quasiparticles.

Two main strategies have been implemented to solve the gGut variational problem, which are discussed in detail in [137]. The first is a direct optimization of the impurity wavefunction amplitudes, together with the Lagrange multipliers, to find the minimum of the energy functional. This approach is generally more robust when additional constraints must be imposed on the ground state [124, 142], such as a fixed magnetization or a fixed particle number, and it will be used explicitly in Chapter 5. A different strategy, presented in [122], consists in promoting, through the introduction of additional Lagrange multipliers, $\hat{\Delta}(\mathbf{R})$ and $\hat{\mathcal{R}}(\mathbf{R})$ to matrices of independent parameters that at the saddle-point correspond to the local single-particle density matrix and the wave function renormalization factors, respectively. This optimization scheme is more convenient when the number of physical/bath orbitals becomes large and the size of the Hilbert space grows exponentially. We use this second approach in the calculations presented in this chapter, where at least six auxiliary orbitals are required to capture the physics of the Hubbard bands of a two-orbital model.

4.2 Topology within the ghost-Gutzwiller formalism

A central object in the gGut formalism is the auxiliary quasiparticle Hamiltonian, built from the renormalized dispersion of the auxiliary quasiparticles (4.14) and the Lagrange multipliers μ_{ab} (4.22) which play the role of a local one-body potential,

$$H_{\text{qp}} = - \sum_{\mathbf{R}\mathbf{R}'} \sum_{ab=1}^{N_{\text{aux}}} \left(\sum_{\alpha\beta=1}^{N_{\text{phys}}} \mathcal{R}_{a\alpha}^\dagger(\mathbf{R}) t_{\mathbf{R}\mathbf{R}'}^{\alpha\beta} \mathcal{R}_{\beta b}(\mathbf{R}') - \mu_{ab}(\mathbf{R}) \delta_{\mathbf{R}\mathbf{R}'} \right) f_{\mathbf{R}a}^\dagger f_{\mathbf{R}'b}. \tag{4.23}$$

We argue that this object is more than a technical intermediate: when the lattice is translationally invariant, the Bloch matrix $H_{\text{qp}}(\mathbf{k})$ provides a genuine band-structure representation of the correlated electronic spectrum, and in particular a natural arena in which the standard tools of noninteracting topological band theory can be applied

to a strongly correlated problem. The goal of this section is to make this statement precise. To do so, we first recall the spectral representation of correlated electrons and the relation between the exact single-particle Green's function and the gGut quasiparticle Hamiltonian, and then discuss how topological invariants are computed in this framework.

4.2.1 Spectral representation of correlated electrons and the gGut Green's function

The single-particle spectrum of a many-body electron system is contained within the single-particle Green's function $G(\omega, \mathbf{k})$, with ω a real frequency and $\mathbf{k}$ a crystal momentum. More generally, $G(z, \mathbf{k})$ is a matrix-valued function of complex frequency z . In this section, we will work on the Matsubara axis, where $z = i\epsilon$ is an imaginary Matsubara frequency, and the interacting Green's function is expressed through the self-energy $\Sigma(i\epsilon, \mathbf{k})$ as

$$G(i\epsilon, \mathbf{k}) = \frac{1}{i\epsilon - H_0(\mathbf{k}) - \Sigma(i\epsilon, \mathbf{k})}, \quad (4.24)$$

with $H_0(\mathbf{k})$ the noninteracting Bloch Hamiltonian.

As discussed at length in Sec. 1.3.1, a few manipulations allow recasting this expression in a form that makes the relation between a general self-energy and Fermi-liquid theory apparent [47, 59, 60]. Following the decomposition of Eq. (1.18), the physical Green's function factorizes as

$$G(i\epsilon, \mathbf{k}) = \sqrt{Z(\epsilon, \mathbf{k})} G_*(i\epsilon, \mathbf{k}) \sqrt{Z(\epsilon, \mathbf{k})}, \quad (4.25)$$

where $G_*(i\epsilon, \mathbf{k}) = [i\epsilon - H_*(\epsilon, \mathbf{k})]^{-1}$ is the quasiparticle Green's function and $Z(\epsilon, \mathbf{k})$ is the positive semi-definite quasiparticle-weight matrix of Eq. (1.19), built from the anti-Hermitian part Σ_2 of the self-energy. The effective, or Fermi-liquid quasiparticle, Hamiltonian $H_*(\epsilon, \mathbf{k})$ was introduced in Eq. (1.21),

$$H_*(\epsilon, \mathbf{k}) = \sqrt{Z(\epsilon, \mathbf{k})} (H_0(\mathbf{k}) + \Sigma_1(i\epsilon, \mathbf{k})) \sqrt{Z(\epsilon, \mathbf{k})}, \quad (4.26)$$

with Σ_1 the Hermitian part of the self-energy; both Z and H_* are even in ϵ . As discussed in Sec. 1.3.2, $H_*(\mathbf{k}) = H_*(\epsilon \rightarrow 0, \mathbf{k})$ is commonly employed in the study of strongly correlated systems as a renormalized one-body effective Hamiltonian to characterize the integrated topology encoded in the Green's function winding number [36, 45–47]. To avoid confusion with H_{qp} in the Gutzwiller formalism, here we will use the term Fermi-liquid quasiparticle Hamiltonian for H_* .

Now, within the gGut approximation we can also access the single-particle Green's function of the lattice system. The standard recipe involves taking the resolvent of the quasiparticle Hamiltonian H_{qp} and projecting it back to the physical space with the renormalization matrices $\hat{\mathcal{R}}$:

$$G_{\alpha\beta}^{\text{gGut}}(i\epsilon, \mathbf{k}) = \sum_{ab} \mathcal{R}_{\alpha a} \left[\frac{1}{i\epsilon - H_{\text{qp}}(\mathbf{k})} \right]_{ab} \mathcal{R}_{b\beta}^\dagger. \quad (4.27)$$

In essence, we build the physical Green's function as a linear combination of the non-interacting, quasiparticle bands. It is in this sense that gGut provides a band structure theory for correlated electrons, and which we will leverage to evaluate topological invariants in the following subsection. While a priori, and despite its shown success [122–124, 143], this prescription may seem somewhat ad hoc, it has been recently shown [125] that in the limit of an infinite number of auxiliary degrees of freedom, the local gGut Green's function becomes equivalent to the local Green's function given by the Dynamical Mean-Field Theory [26], which is known to be exact in the infinite-coordination limit.

Furthermore, we now show how the gGut Green's function in Eq. (4.27) can be interpreted as a finite truncation of the Lehmann expansion of the exact Green's function, within a local embedding approximation. To do so, we first recall that we can always split the positive semi-definite matrix $Z(\epsilon, \mathbf{k})$ as

$$Z(\epsilon, \mathbf{k}) = A(\epsilon, \mathbf{k}) A^\dagger(\epsilon, \mathbf{k}), \quad (4.28)$$

where in principle $A(\epsilon, \mathbf{k})$ can be a rectangular matrix with a number of rows N equal to the number of physical orbitals, but a larger number of columns M . With this, the Fermi-liquid quasiparticle Hamiltonian H_* in Eq. (4.26) follows

$$H_*(\epsilon, \mathbf{k}) \rightarrow A^\dagger(\epsilon, \mathbf{k}) (H_0(\mathbf{k}) + \Sigma_1(i\epsilon, \mathbf{k})) A(\epsilon, \mathbf{k}), \quad (4.29)$$

becoming an $M \times M$ Hermitian matrix. Consequently, the physical, interacting one-body Green's function can also be rewritten in terms of the rectangular $A(\epsilon, \mathbf{k})$ matrices as

$$G(i\epsilon, \mathbf{k}) = A(\epsilon, \mathbf{k}) \frac{1}{i\epsilon - H_*(\epsilon, \mathbf{k})} A^\dagger(\epsilon, \mathbf{k}). \quad (4.30)$$

At first glance, there seems to be no point in choosing $M > N$, hence a number of quasiparticles larger than the number of physical orbitals. However, inspecting Eq. (4.30), it becomes apparent that such a strategy can lead to an important simplification: if M is large enough, it should become possible to approximate the full $G(i\epsilon, \mathbf{k})$ with frequency-independent $A(\mathbf{k})$ and $H_*(\mathbf{k})$, namely

$$G(i\epsilon, \mathbf{k}) \simeq A(\mathbf{k}) \frac{1}{i\epsilon - H_*(\mathbf{k})} A^\dagger(\mathbf{k}). \quad (4.31)$$

After all, for M going to infinity, this is always true as can be seen inspecting the Lehmann representation of the Green's function

$$G_{\alpha\beta}(i\epsilon, \mathbf{k}) = \sum_n \left(\frac{\langle n | c_{\alpha\mathbf{k}} | 0 \rangle \langle 0 | c_{\beta\mathbf{k}}^\dagger | n \rangle}{i\epsilon - (E_0 - E_n)} + \frac{\langle 0 | c_{\alpha\mathbf{k}} | n \rangle \langle n | c_{\beta\mathbf{k}}^\dagger | 0 \rangle}{i\epsilon - (E_n - E_0)} \right), \quad (4.32)$$

where α, β label the physical orbitals as before and n the many-body eigenstates. If we now define

$$A_{\alpha n}(\mathbf{k}) = \begin{cases} \langle n | c_{\alpha\mathbf{k}} | 0 \rangle & \text{if } \epsilon_n(\mathbf{k}) = E_0 - E_n < 0, \\ \langle 0 | c_{\alpha\mathbf{k}} | n \rangle & \text{if } \epsilon_n(\mathbf{k}) = E_n - E_0 > 0, \end{cases} \quad (4.33)$$

then the Green's function can be written as

$$G_{\alpha\beta}(i\epsilon, \mathbf{k}) = \sum_n A_{\alpha n}(\mathbf{k}) \frac{1}{i\epsilon - \epsilon_n(\mathbf{k})} A_{\beta n}^*(\mathbf{k}), \quad (4.34)$$

where the number of columns of $A_{\alpha n}(\mathbf{k})$ grows exponentially with the system size, as the number of many-body states labeled by n . Identifying $A(\mathbf{k}) \equiv R(\mathbf{k})$, we almost arrive at the gGut approximation for the Green's function in Eq. (4.27). The only missing step is to justify the removal of the formal momentum dependence of the projection matrices in Eq. (4.31). This can be interpreted as a local, hence $\mathbf{k}$ -independent, approximation, which becomes natural considering the infinite-coordination limit implicit in the Gutzwiller approximation. Thus, the gGut approximation to the Green's function in Eq. (4.27) can be seen as a finite truncation of the Lehmann expansion to the exact Green's function within a local approximation. Armed with this, we can tackle the extraction of topological invariants from this band-structure representation of strongly correlated electrons.

We note that pole-expansion based expressions have been explored in the context of correlated topology [144–147]. These typically are constructed as few-pole approximations to an otherwise computed self-energy, e.g. through DMFT. In contrast, we stress that the pole-expansion of the Green's function in gGut, and thus the quasiparticle band description, is naturally built into the ansatz: the position and bandwidths of the ghost bands are fixed through the variational principle.

4.2.2 Topological invariants within ghost-Gutzwiller

We are finally ready to examine how the band-structure emerging from $H_{\text{qp}}(\mathbf{k})$ can be used to extract the topological invariants of the system. Specifically, following the previous discussion on spectral representations of correlated electrons, we demonstrate the physical relevance of computing Chern numbers for these quasiparticle bands, and their relation to the Chern number of the fully interacting system.

To this end, we note that the gGut Green's function introduced in Eq. (4.27) embodies the notion that the quasiparticle Hamiltonian, although optimized to describe ground-state properties, nonetheless provides a meaningful approximation to single-particle excitations. This perspective becomes even more compelling when considering the robust quantization of topological invariants of the ground state. The energy- and momentum-resolved features of the approximate single-particle excitations in $H_{\text{qp}}(\mathbf{k})$ are expected to be protected by the intrinsic robustness of the topological invariants they support. In this sense, it is reasonable to expect that $H_{\text{qp}}(\mathbf{k})$ in Eq. (4.23) should properly describe the topological features of the original, interacting system. It is instructive to work out this description in a particular example, and thus the rest of this subsection is devoted to explicitly establishing the connection between the gGut quasiparticle Hamiltonian and the winding number of the physical Green's function, a central quantity in the description of ground state topology in self-energy based

methods like DMFT.

In Sec. 1.3.2, we introduced the winding number of the single-particle Green's function as [45–47]

$$W[G] = \frac{1}{24\pi^2} \int d\epsilon d\mathbf{k} \epsilon_{\mu\nu\rho} \text{Tr} \left(G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\rho G^{-1} \right), \quad (4.35)$$

where $G \equiv G(i\epsilon, \mathbf{k})$, the indices μ, ν, ρ run over the three coordinates (ϵ, k_x, k_y) with $\partial_0 \equiv \partial_\epsilon$ and $\partial_{1,2} \equiv \partial_{k_{x,y}}$, $\epsilon_{\mu\nu\rho}$ is the antisymmetric tensor, and the frequency integral runs along the whole imaginary axis. When perturbation theory holds, $W[G]$ coincides with the zero-temperature Hall conductance in units of $e^2/2\pi\hbar$ [36, 45–47]. This makes the winding number a particularly powerful tool for methods that grant access to the full single-particle Green's function, such as DMFT and gGut. However, the direct evaluation of Eq. (4.35) is often computationally expensive. A common alternative is to exploit the fact that this winding number is equivalent to the Chern number of the Hermitian matrix $-G(0, \mathbf{k})^{-1}$ [63], or equivalently $-G_*(0, \mathbf{k})^{-1}$ [47], which is related to the Fermi-liquid quasiparticle Hamiltonian in Eq. (4.26).

We mentioned that within the gGut framework the physical single-particle thermal Green's function $G(i\epsilon, \mathbf{k})$, which is an $N \times N$ matrix, is approximated by

$$G(i\epsilon, \mathbf{k}) \approx G^{\text{gGut}}(i\epsilon, \mathbf{k}) = \hat{\mathcal{R}} G_{\text{qp}}(i\epsilon, \mathbf{k}) \hat{\mathcal{R}}^\dagger, \quad (4.36)$$

where

$$G_{\text{qp}}(i\epsilon, \mathbf{k}) = \frac{1}{i\epsilon - H_{\text{qp}}(\mathbf{k})},$$

is the $M \times M$ quasiparticle Green's function matrix with $M \geq N$. It can be shown [148] that the winding number of $G^{\text{gGut}}(i\epsilon, \mathbf{k})$ is equal to that of $G_{\text{qp}}(i\epsilon, \mathbf{k})$, as long as the matrix $\hat{\mathcal{R}}$ is momentum independent:

$$W[G] \approx W[G^{\text{gGut}}] = W[G_{\text{qp}}] \quad (4.37)$$

The winding number of $G_{\text{qp}}(i\epsilon, \mathbf{k})$ can be straightforwardly computed from the Chern number of the occupied quasiparticle bands of $H_{\text{qp}}(\mathbf{k})$, which is a standard procedure in noninteracting topological band theory. This establishes a direct link between the topological invariants of the interacting system and the Chern numbers of the gGut quasiparticle bands, providing a practical and computationally efficient method to evaluate topological properties in strongly correlated systems.

We conclude by stressing that $H_{\text{qp}}(\mathbf{k})$ can provide even more topological information than merely the winding number Eq. (4.35). The latter is, in fact, an integrated quantity that does not convey information about the energy and momentum resolved topological features useful for interpreting experimental spectra. Conversely, the quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$ in gGut offers this information as well without any additional computational cost. This feature grants access to a band structure that, unlike DFT, also encompasses the Hubbard bands, and thus enables a direct comparison with experimental data under the assumption that the quasiparticle bands accurately represent the genuine single-particle spectrum.

4.3 Benchmarks and quasiparticle perspective

In this chapter we use the half-filled interacting BHZ model, introduced in Sec. 1.1, to validate the gGut quasiparticle-band framework in a setting where band topology and local correlations are both essential. This model has been extensively studied with DMFT and extensions [30, 34, 49, 54, 55, 76, 149], providing established reference results for both correlation indicators (effective-mass renormalization) and topological indices. Here we focus on two standard correlation-driven effects in the phase diagram depicted in Fig. 1.2a: the renormalized quantum spin Hall insulator (QSHI) to trivial band insulator (BI) transition, and the correlation-driven transition from the QSHI to a Mott insulator (MI). To enable a direct, parameter-matched comparison, we complement the existing literature with our own single-site DMFT calculations. The latter were performed using the impurity solver implemented in the TRIQS library [71], employing a continuous-time quantum Monte Carlo algorithm based on a hybridization expansion of the partition function [72, 73]. The DMFT calculations were performed at inverse temperature $\beta = 1/T = 50$ ($k_B = 1$), in units of the hopping amplitude t , and the results shown in this chapter show no dependence upon further lowering the temperature: thus we can safely use them to benchmark the gGut data obtained at $T = 0$.

Before specifying the local interaction parameters used in this section, a brief comment on the form of the interaction Hamiltonian is in order. The interaction considered in this chapter differs slightly from the one introduced in Eq. (1.11): in the dipole component $H_{\text{dip}}(\mathbf{R})$ (1.12), the Ising-like term $J S_s^z S_p^z$ is replaced by its $SU(2)$ -symmetric form $J \vec{S}_s \cdot \vec{S}_p$, thereby recovering the standard Hubbard-Kanamori interaction [64]. This choice was dictated by our numerical gGut implementation, which was built assuming $SU(2)$ -symmetric local interactions. The latter is not a limitation of the method, and the Ising-like term can be easily implemented as well. This change mainly affects the strong coupling atomic limit, where the lowest energy two-electron configuration of $H_{\text{int}}(\mathbf{R})$ becomes the threefold-degenerate $S = 1$ triplet rather than the $S_z = \pm 1$ doublet selected by the Ising-like term. We have explicitly verified that this change does not impact the results discussed in this chapter, as long as one does not probe excitonic instabilities or the magnetic ordering of the Mott insulating phase, where the difference between the two forms becomes physically relevant. The interaction parameters in Eq. (1.11) chosen for this section are $U_s = U_p \equiv U$, $V = U - 2J$ and $J = U/4$. Moving to the analysis of the results shown in Fig. 4.1, we can see that in the weakly correlated regime the primary role of the interaction is to shift the topological transition between the QSHI and the BI towards higher values of the on-site bare mass M . Within the gGut framework the QSHI–BI transition is signaled by a closure and reopening of the gap of the quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$, i.e. by a band inversion at the critical value M_c (we recall that in the non-interacting case $M_c = 2$). While in the trivial BI phase the valence and conduction bands of $H_{\text{qp}}(\mathbf{k})$ have a dominant p - and s -like character ($n_p - n_s \simeq 1$ in the GS), respectively, in the QSHI phase the

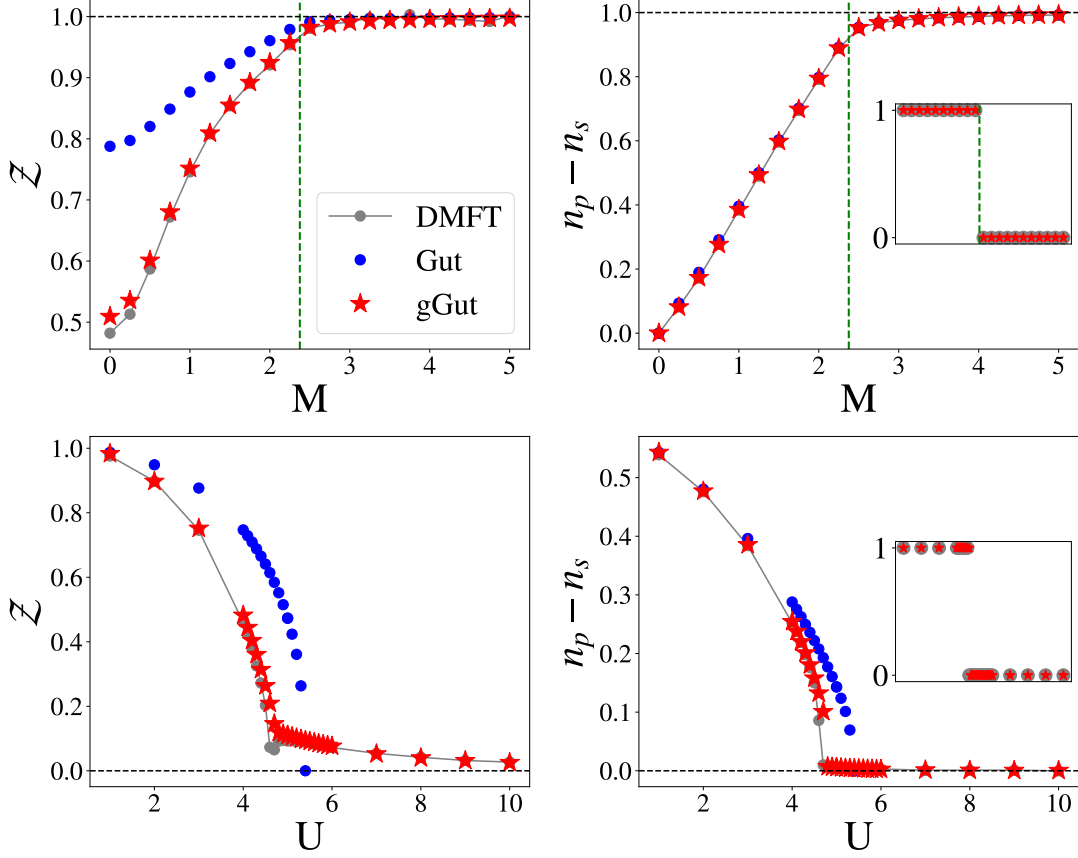


Figure 4.1: Comparison between different methods on two representative cuts of the phase diagram. Upper panels: quasiparticle residue $\mathcal{Z}$, related to the effective-mass enhancement $m^*/m \sim 1/\mathcal{Z}$, and on-site orbital polarization $n_p - n_s$ at fixed $U = 3.0$, as a function of the bare mass M . The inset in the right plot shows the quantized topological invariants computed within gGut and DMFT. The green dashed line marks the topological transition between the QSHI and the BI phases. Lower panels: same analysis at fixed $M = 1.0$, across the transition from the QSHI to the MI as a function of the interaction strength U .

orbital character of the low-energy bands is mixed ($n_p - n_s < 1$). In the parameter range considered here, the gap closes via a linear (Dirac) band crossing of the quasiparticle bands. Accordingly, the QSHI–BI boundary discussed in Fig. 4.1 corresponds to a continuous topological band-inversion transition [150]. At fixed $U = 3$ the transition happens at the renormalized value $M_c \simeq 2.3$. Already the conventional Gutzwiller (Gut) solution without ghosts can accurately capture the behavior of the on-site orbital polarization $n_p - n_s$; nonetheless it severely underestimates the role of the correlations quantified, e.g., by the quasiparticle renormalization matrix Z defined as

$$Z \equiv \left(1 - \frac{\partial \text{Re} \Sigma(\omega)}{\partial \omega} \bigg|_{\omega \rightarrow 0} \right)^{-1}, \quad (4.38)$$

with ω a real frequency. We remark that Z is diagonal thanks to the symmetries of the local Green’s function and self-energy: $Z = \mathcal{Z} \otimes \mathbb{I}_{4 \times 4}$, where $\mathcal{Z}$ is related to the

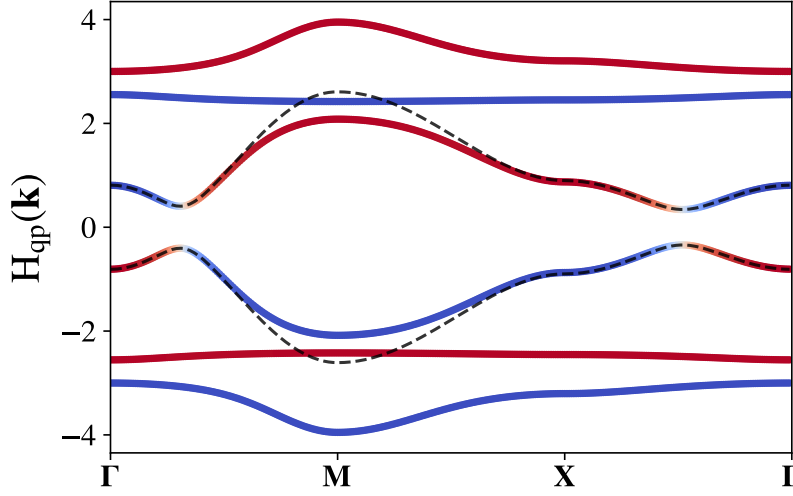


Figure 4.2: Band structure of the quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$ along a high-symmetry path in the Brillouin zone, at $M = 1.5$ and $U = 3.0$. The color scale indicates the orbital character of the eigenstates: red for s -like and blue for p -like contributions. The two energy bands close to the Fermi level have a mixed-orbital character and are topologically nontrivial. In contrast, the high-energy bands, associated with the dispersive Hubbard bands, are topologically trivial. For comparison, black dashed lines show the dispersion of $H_*(\mathbf{k}) = \sqrt{Z} (H_0(\mathbf{k}) + \text{Re } \Sigma(0, \mathbf{k})) \sqrt{Z}$, which encodes the topological content of the Green's function winding number.

effective-mass enhancement $m^*/m \sim 1/Z$.

By contrast, just including two ghosts per orbital in the quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$, the gGut solution can accurately describe correlation effects, matching the DMFT predictions.

In the inset of the right plots of Fig. 4.1, we also see perfect agreement between the topological invariant computed from $H_{\text{qp}}(\mathbf{k})$, using the standard Thouless-Kohmoto-Nightingale-den Nijs (TKNN) formula [6] for independent electrons, and the winding number of the Green's function obtained in DMFT.

Focusing now on a cut of the phase diagram at fixed M and varying U , we can drive the system towards a strongly correlated Mott insulator (MI). The Gut solution correctly describes the qualitative renormalization of the low-energy bands of the QSHI before the onset of the MI, but it fails to faithfully describe the Mott insulating phase. This is a consequence of what is observed in the Mott transition in a single-band Hubbard model at half-filling [151]: the Gutzwiller ansatz satisfactorily accounts for the narrowing and eventual vanishing of the coherent metallic band at the Fermi level, but it fails to describe the incoherent high-energy Hubbard bands, which characterize the nature of the insulating state and relate it to the atomic limit. Only the inclusion of the ghosts allows for a meaningful description of the MI, which closely agrees with the DMFT solution as shown in the bottom panels of Fig. 4.1. In the predicted MI phase

the integrated topology encoded in the winding number is trivial, consistently with the fact that the zeros of the Green's function are flat and trivial [47] in any local approximation. This should be contrasted with the non-trivial topology that the zeros of the Green's function can acquire on a MI, discussed in Chapter 1, where a DCA treatment beyond DMFT endows the bands of zeros with a genuine dispersion.

We conclude this section with a closer inspection of the band structure arising in gGut from the quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$ of the auxiliary fermionic degrees of freedom. In Fig. 4.2, we show the eigenvalues of $H_{\text{qp}}(\mathbf{k})$ for the correlated QSHI phase at $M = 1.5$ and $U = 3.0$. The color code reflects the s - and p -orbital character of the corresponding Bloch eigenstates. The two energy bands close to the Fermi level are topologically nontrivial, as suggested by their mixed-orbital character and confirmed from the calculation of the spin-resolved Chern number. In contrast, the high-energy bands, associated with the dispersive Hubbard bands, are topologically trivial in this case, but a more detailed discussion about their topological character and physical implications is deferred to Sec. 4.5. For comparison, we also show the eigenvalues of $H_*(\mathbf{k})$ (dashed black lines), which encodes the topological content of the Green's function winding number in Eq. (4.35). As shown in the figure, the low-energy bands of $H_{\text{qp}}(\mathbf{k})$ closely match those of $H_*(\mathbf{k})$, particularly near the avoided crossing where the Berry curvature is concentrated. When perturbation theory is valid, both approaches yield consistent information about the topological nature of the system as encoded by the Green's function winding number. However, while $H_*(\mathbf{k})$ is intrinsically tied to the winding number description, $H_{\text{qp}}(\mathbf{k})$ also captures high-energy excitations, including the Hubbard bands and their possible topological features. This establishes $H_{\text{qp}}(\mathbf{k})$ as a general and physically grounded tool for analyzing the topology of excited states throughout the spectrum of strongly correlated systems, complementing the successful topological Hamiltonian approach and setting the stage for the analysis of topological Hubbard bands in the next sections.

4.4 OBC calculations and edge states in the quasiparticle Hamiltonian

An equivalent and more direct way to characterize the band topology of a system is to look for symmetry-protected edge states under open boundary conditions (OBC) along one direction. According to the bulk-edge correspondence [152, 153], gapless edge states must emerge at the interface between regions belonging to different topological phases, i.e. characterized by distinct topological invariants. However, solving the full many-body problem on a large, finite-size system is numerically prohibitive. A computationally efficient alternative is to study a two-dimensional slab geometry, decomposing it as a set of coupled one-dimensional chains. Inter-chain couplings are fully retained in the slab Hamiltonian, while electronic correlations are treated at the single-impurity (local) level with parameters that may depend on the chain index y .

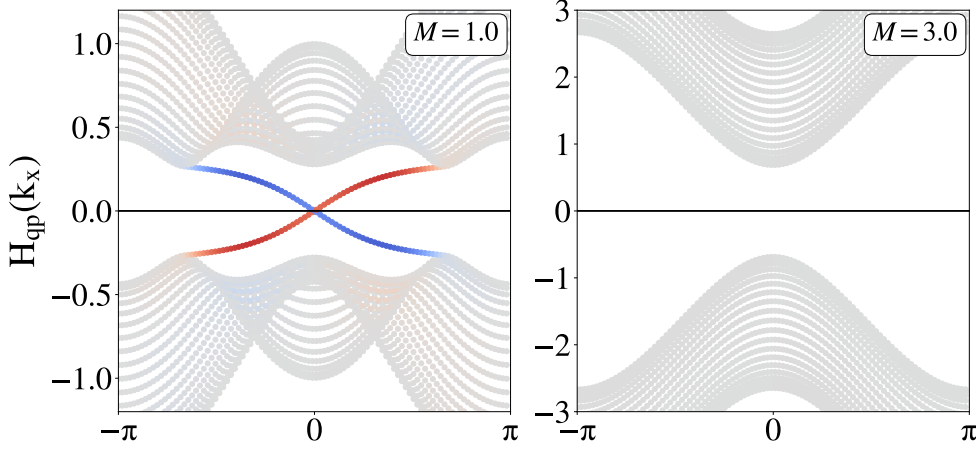


Figure 4.3: Quasiparticle spectrum of $H_{\text{qp}}(k_x)$ for a slab geometry with OBC along $\hat{y}$ ($N_y = 20$) and PBC along $\hat{x}$. We show the data for two representative points of the phase diagram cut discussed in the upper panels of Fig. 4.1 ($U = 3.0$). The color code quantifies the degree of localization of the spin-up eigenstates at the upper (blue) and lower (red) edges (for the spin-down sector the colors are reversed, as expected for helical edge states). In the topological phase, edge states emerge within the bulk gap and cross the chemical potential, consistent with the nontrivial Chern number of $H_{\text{qp}}(\mathbf{k})$ and the bulk-boundary correspondence.

Consequently, one impurity problem is solved for each inequivalent chain, and the total computational cost scales linearly with the number of chains N_y , assuming the impurity solver is the main bottleneck. Although the impurity problems are solved separately, they are coupled through the embedding, which is built from the full slab quasiparticle Hamiltonian H_{qp} , including inter-chain hopping. Crucially, the impurity problem arising in the gGut embedding scheme is much cheaper than the analogous one in approaches like DMFT, enabling the exploration of larger system sizes. This opens the door to studying the interplay between correlations, topology, and finite-size effects in regimes that have so far been explored mostly in noninteracting systems [56, 154].

In Fig. 4.3 we show the quasiparticle spectrum of $H_{\text{qp}}(k_x)$ for a slab geometry with open boundaries along $\hat{y}$ ($N_y = 20$) and periodic boundary conditions (PBC) along $\hat{x}$. The calculations were performed for two values of M , corresponding to representative points along the fixed $U = 3.0$ cut of the phase diagram discussed in Sec. 4.3 (see Fig. 4.1). For each value of k_x , there are $N_{\text{orbitals}} \times N_{\text{ghosts}} \times N_y$ eigenvalues and eigenstates per spin. In the topologically nontrivial phase, we observe two helical edge states crossing the chemical potential within the bulk gap. These edge states are exponentially localized at the boundaries, as highlighted by the color coding. Their finite spectral weight in the physical density of states further supports the interpretation of the Chern numbers computed from the occupied bands of $H_{\text{qp}}(\mathbf{k})$ as a genuine topological invariant of the interacting system.

By extending this slab analysis to multiple fixed M cuts of the phase diagram, we can observe a nontrivial and, to the best of our knowledge, never explored manifestation of

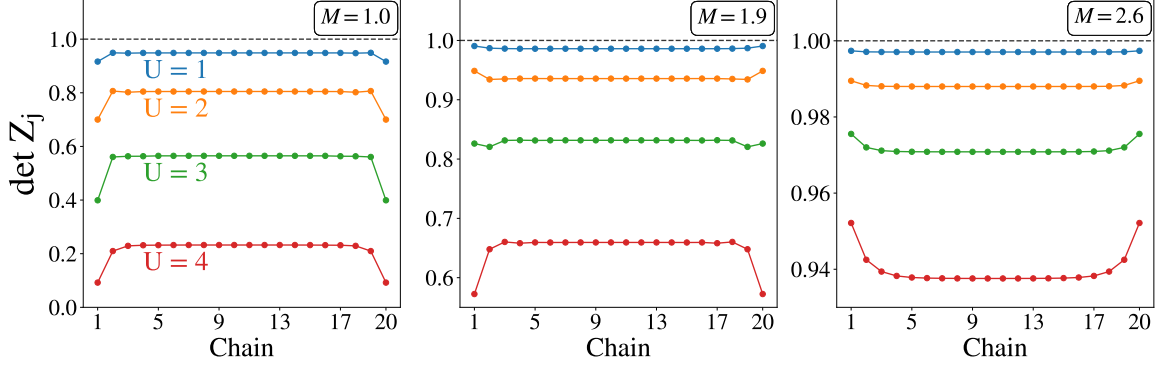


Figure 4.4: Determinant of the quasiparticle residue matrices Z_j for each chain j , for a slab geometry with OBC along $\hat{y}$ ($N_y = 20$) and PBC along $\hat{x}$. Each panel shows results for four values of the interaction strength U , at fixed M . At the slab boundaries, the reduced hopping due to the interface with the vacuum modifies the local correlations: depending on whether the dominant effect is the effective enhancement of the interaction strength or the increase in the effective mass-to-hopping ratio $M_{\text{eff}}/t_{\text{eff}}$, correlations may be either enhanced or suppressed. In the latter case, the boundaries become effectively “less topological” and thus less correlated by the interaction.

the interplay between topology, interactions and boundary effects. Before proceeding, it is important to note that in the OBC geometry, the wavefunction renormalization matrix Z_j , with j indexing the chains, is no longer diagonal in the orbital basis. This is due to the absence of the symmetry constraints that, under PBC, enforce both the local Green’s function and the self-energy to be orbital-diagonal. These off-diagonal elements become significant near the boundaries of a strongly correlated QSHI, but decay rapidly within the bulk. For this reason, in Fig. 4.4, we plot the determinant of the quasiparticle residue matrix Z_j , rather than only the diagonal elements as in the PBC case. We emphasize, however, that both the determinant and the diagonal entries exhibit the same chain-dependent behavior, which we now discuss.

In the first panel of Fig. 4.4, we show the spatial profile of $\det Z_j$ across the slab at fixed $M = 1.0$, as a function of the chain index j , for several values of the interaction strength U . The boundary chains exhibit stronger renormalization (smaller Z_j) than the bulk, indicating enhanced correlations. This is expected, as the reduced kinetic energy at the edges, due to missing neighbors, leads to a relatively stronger effect of the interaction. Interestingly, for $M = 1.9$, we find the opposite behavior at small U : correlations are suppressed at the boundaries. This counterintuitive result arises because the reduced hopping at the edges increases the effective ratio $M_{\text{eff}}/t_{\text{eff}}$, thereby favoring a topologically trivial phase. As a result, the boundaries are effectively “less topological” and hence less correlated by the interaction. Only at larger U does the usual trend of enhanced edge correlations re-emerge. Finally, the third panel of Fig. 4.4 shows the spatial dependence of $\det Z_j$ for $M = 2.6$, which further supports our argument: here the dominant contribution comes from the renormalization of $M_{\text{eff}}/t_{\text{eff}}$ at the edges, and therefore the edge renormalization is reversed compared to the $M = 1.0$ case. These

results clearly demonstrate how the competition between topological and correlation effects leads to nontrivial boundary behavior in interacting topological insulators.

4.5 Topology of the Hubbard bands and their interplay with magnetism

We now turn to the investigation of the topology associated with high-energy excitations, such as the lower (LHB) and upper (UHB) Hubbard bands of an interaction-driven MI, as captured by the quasiparticle Hamiltonian $H_{\text{qp}}(\mathbf{k})$. To isolate this effect, we consider the simplest realization of a MI phase in the interacting BHZ model considered here. We thus set the interaction parameters in (1.11) as $U_s = U_p = 8$, $V = 0$ and $J = 0$. Under these conditions, the system reduces to two copies of a single-band Hubbard model in the Mott insulating regime, weakly coupled by the noninteracting hybridization hopping terms between the orbitals that open the topologically nontrivial gap. This setup allows us to explore the topological character of the Hubbard bands and their interplay with the underlying band topology of the noninteracting model.

In Fig. 4.5 we show the band structure of $H_{\text{qp}}(\mathbf{k})$ for three representative values of the on-site bare mass M , both in PBC and OBC. The resulting quasiparticle band structure exhibits two hallmark features of the gGut description of a MI:

- (i) a flat band at the Fermi level for each orbital, corresponding to the auxiliary fermionic degree of freedom that mimics the narrow metallic peak in the interacting density of states (DOS). Since this band carries no weight in the physical DOS of the insulator ($\mathcal{R} \rightarrow 0$), its dispersion also vanishes;
- (ii) a pair of Hubbard bands per orbital, which encode the high-energy charge excitations of the system.

Notably, for $M \lesssim 1$, the Hubbard bands associated with the two orbitals hybridize, develop a mixed orbital character, and open a high-energy gap. The color scale indicates the orbital polarization of each band, highlighting regions where band inversion occurs. For this regime the spin-resolved Chern numbers of the ghost bands also signal a nontrivial topology. According to the bulk-boundary correspondence, this should result in helical edge states confined within the gaps of the lower and upper Hubbard bands when the system is placed in an open geometry. In the lower panels of Fig. 4.5 we confirm this by showing the eigenvalue spectrum of $H_{\text{qp}}(k_x)$ for a slab geometry with OBC along $\hat{y}$ ($N_y = 20$) and PBC along $\hat{x}$. As expected, for $M \lesssim 1$, two pairs of edge states emerge in the high-energy topological gaps. The color scale again quantifies the spatial localization of these states at the boundaries, confirming their edge character. We note that the gap closing/opening visible in the high-energy Hubbard-like bands corresponds to a finite-energy band touching among poles of $H_{\text{qp}}(\mathbf{k})$. This feature reflects the reorganization of spectral poles/weights and should not be conflated with the ground-state topological transition, which is determined by the quasiparticle gap at the Fermi level.

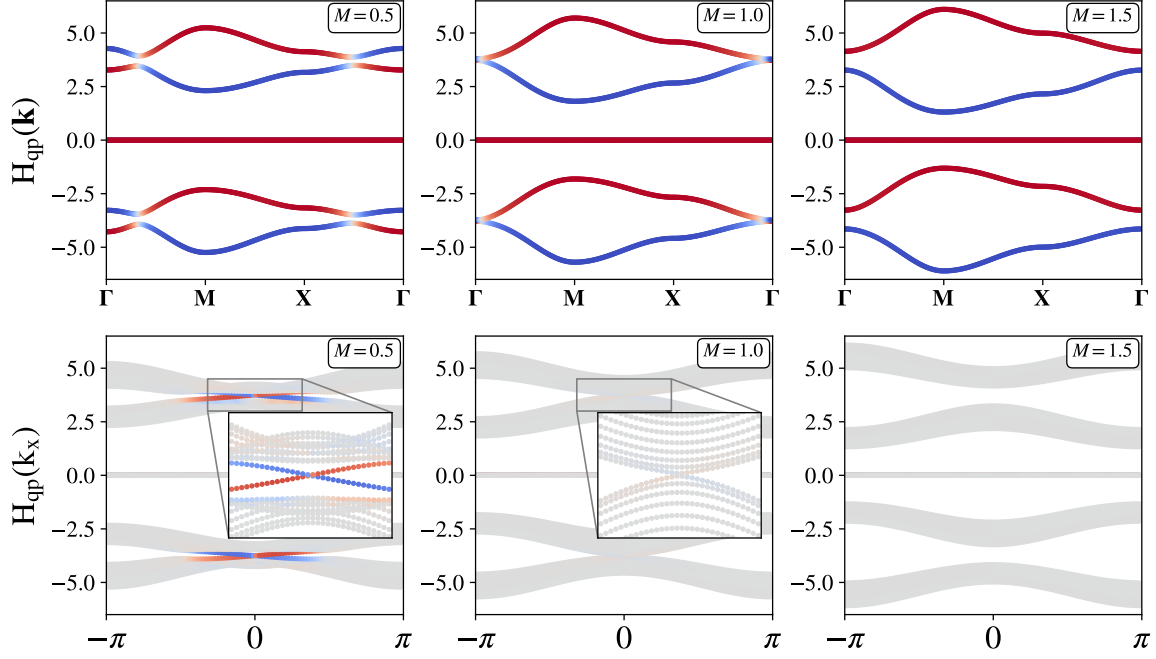


Figure 4.5: Quasiparticle band structure of $H_{\text{qp}}(\mathbf{k})$ showing the topological Hubbard bands. Upper panels: PBC band structures at $U = 8.0$ and for three values of M . The color scale indicates the orbital polarization (red for s and blue for p orbital), highlighting the hybridization and band inversion between the Hubbard bands. Lower panels: spin-up eigenvalues of $H_{\text{qp}}(k_x)$ in a slab geometry with OBC along $\hat{y}$ ($N_y = 20$). The color code quantifies the degree of localization of the spin-up eigenstates at the upper (blue) and lower (red) edges (for the spin-down sector the colors are reversed), revealing the emergence of topologically protected helical edge states inside the Hubbard band gaps for $M \lesssim 1$.

An intriguing aspect of our results is the value of M for which we observe the topological transition between the Hubbard bands. Specifically, we observe that the transition occurs around $M \approx M_c/2 = 1$, where M_c is the critical mass that marks the topological phase transition in the noninteracting model. We can rationalize this result by assuming that, well inside the MI, the self-energy is well approximated by

$$\Sigma(i\epsilon) \simeq \frac{\Delta^2}{i\epsilon - M\sigma_0 \otimes \tau_3} + \frac{U}{2}\sigma_0 \otimes \tau_0, \quad (4.39)$$

the first term originating from an expansion around the atomic limit with Δ proportional to the Mott gap, and the second accounting for the Hartree-Fock shift. At half-filling, this Hartree-Fock term exactly compensates the chemical potential, and the retarded single-particle Green's function reads

$$G(\omega + i0^+, \mathbf{k}) = \frac{1}{\omega - H_0(\mathbf{k}) + \mu - \Sigma(\omega + i0^+) + i0^+}. \quad (4.40)$$

Solving for the poles yields the condition

$$\omega - H_0(\mathbf{k}) - \frac{\Delta^2}{\omega - M\sigma_0 \otimes \tau_3} = 0, \quad (4.41)$$

which, at leading order in $\Delta \gg 1$, gives the Hubbard band dispersions

$$\omega_{\pm} = \frac{H_0(\mathbf{k}) + M\sigma_0 \otimes \tau_3}{2} \pm \Delta. \quad (4.42)$$

In the resulting dispersion of the Hubbard bands, the effective hopping amplitudes are reduced by a factor of two with respect to the bare dispersion ones, while the effective M remains approximately the same. Their band inversion is thus expected to occur when $M_{\text{eff}}/t_{\text{eff}} = M/(t/2) \approx M_c/t$. This scaling explains the emergence of a topological transition in the Hubbard bands at $M \approx M_c/2$. As highlighted in the approximate analytic argument, this shift is a genuinely nonperturbative feature of the high-energy spectrum in the Mott insulating regime, and is fully captured within the gGut framework.

It is worth noting that a topological classification of MIs has also been proposed based on the structure of the zeros of the Green's function [36, 47, 55, 61, 155]. When nonlocal dynamical correlations are included—beyond what is accessible in single-site DMFT or gGut—dispersive zeros emerge within the Mott gap. As we discussed in Chapter 1, this is precisely what happens in a cluster (DCA) treatment of an interacting BHZ model, where such zeros can acquire a topologically nontrivial structure and contribute to a finite winding number of the Green's function itself. Importantly, the existence of zeros within the Mott gap reflects the underlying structure of the Green's function as a sum of contributions from the LHB and UHB poles; the presence of a pair of poles generically implies a zero in between. This observation suggests that, at least at leading order, the topology of the Hubbard bands and the topology of Green's function zeros may originate from a common non-perturbative mechanism. Further exploration of this potential link could shed light on how local and nonlocal correlations cooperate in defining the topological structure of interacting systems. A detailed analysis will require cluster extensions of gGut that incorporate nonlocal correlation effects, which we leave for future studies.

4.5.1 Interplay between topology, magnetism and correlation

Given the interpretability of our framework, it presents particular promise to aid in the design of novel materials with unexplored topological properties. In recent years, leveraging the interplay between topology and magnetism has emerged as a fruitful direction [156–158], and we expect the gGut formalism to provide meaningful insights in this field. To illustrate this, we consider the MI with topological Hubbard bands discussed above, and build upon the magnetic response of the paramagnetic Mott insulator, previously explored in [130, 159], to investigate how a magnetic field affects the topology of the high-energy Hubbard bands.

To this end, we probe the magnetic response of a MI by applying a small and uniform magnetic field to the lattice to induce a finite magnetization at each site. Thus, the

magnetic susceptibility χ is defined as

$$\chi = \left. \frac{\partial m}{\partial h} \right|_{h \rightarrow 0}, \quad (4.43)$$

where m is the magnetization per site and h is the applied magnetic field. In a conventional band insulator, where both charge and spin excitations are gapped, the magnetic susceptibility vanishes as $T \rightarrow 0$. By contrast, the Mott insulator displays a Pauli-like magnetic susceptibility that remains finite at zero temperature, despite the presence of a charge gap. This behavior is correctly captured by the paramagnetic gGut solution, although doing so requires some care in treating the magnetic response when the associated impurity problem has a degenerate ground state. As discussed above, there are two possible ways to solve the gGut equations and minimize the energy functional. One possibility is to parametrize the most general impurity wavefunction compatible with a paramagnetic insulating state. Minimizing the energy with respect to all variational parameters then correctly yields a finite magnetization in the Mott-insulating phase once a finite magnetic field is applied. Alternatively, it is often more convenient to work in the embedding formulation, where the quasiparticle and impurity problems are solved separately and self-consistently, as we have done in this work. In this formulation, however, the impurity ground state at $h = 0$ is degenerate: it can be written as an arbitrary linear combination of the lowest singlet and triplet configurations of the impurity model. An infinitesimal magnetic field would then select a particular combination in this degenerate manifold, fully polarizing the impurity problem and thereby incorrectly predicting a fully polarized lattice state with $m = 1$ for arbitrarily small h . To avoid this artifact, we have shown in related work [142] that the ferromagnetic response can instead be accessed by fixing the magnetization on the impurity site. This procedure effectively selects the appropriate linear combination of the two lowest-energy impurity eigenstates¹. It is physically equivalent to probing the system in a magnetic field, while bypassing the ambiguity associated with the degenerate impurity ground state. Moreover, it allows us to compute the ground-state energy as a function of the magnetization, $E(m)$. The magnetic susceptibility then follows directly from the curvature of $E(m)$ around $m = 0$, as we now show. The energy as a function of the magnetic field $E(h)$ can be obtained from a Legendre transform of $E(m)$, as

$$E(h) = \min_m (E(m) - hm) = E(\bar{m}) - h\bar{m} \quad (4.44)$$

where $\bar{m}$ is the value of the magnetization that minimizes the expression in parentheses, thus $\partial_m E(m)|_{\bar{m}} = h$. It follows then

$$\begin{aligned} \partial_h E(h) &= (\partial_h m \partial_m E(m) - m - h \partial_h m) |_{\bar{m}} \\ &= \partial_h m (\partial_m E(m) - h) |_{\bar{m}} - \bar{m} \\ &= -\bar{m}, \end{aligned} \quad (4.45)$$

¹In the $h=0$ limit, these correspond to degenerate singlet and triplet configurations.

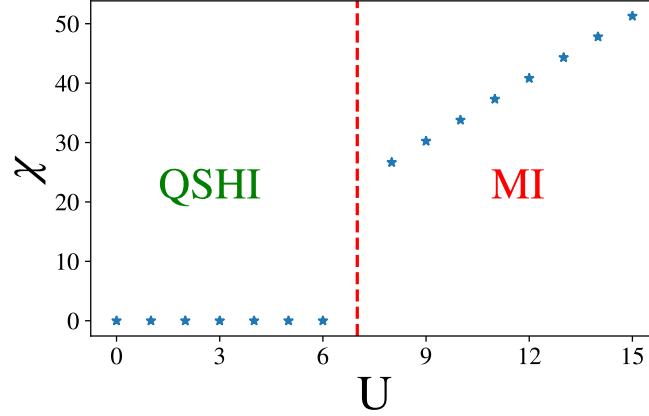


Figure 4.6: Magnetic susceptibility χ as a function of the interaction strength U , for fixed $M = 1.0$. The red dashed line marks the transition between the two insulating phases. In the QSHI phase, χ vanishes, consistent with the gapped nature of the insulating state. In contrast, the MI phase exhibits a finite susceptibility that increases as $\chi \sim U$. This paramagnetic behavior suggests the presence of gapless quasiparticles inside the gap with their own Fermi surface.

so that

$$\begin{aligned} \partial_h \bar{m}|_{h \rightarrow 0} &= -\partial_h^2 E(h)|_{h \rightarrow 0} \\ &= -\left(\partial_h^2 m (\partial_m E(m) - h) + (\partial_h m)^2 \partial_m^2 E(m) - 2\partial_h m \right)|_{\bar{m}, h \rightarrow 0} \end{aligned} \quad (4.46)$$

and the magnetic susceptibility can be obtained from the curvature of $E(m)$ at $m = 0$ as

$$\chi = \partial_h \bar{m}|_{h \rightarrow 0} = \left(\partial_m^2 E(m) \right)_{\bar{m} \rightarrow 0}^{-1}. \quad (4.47)$$

Examining the magnetic susceptibility, shown in Fig. 4.6, we find that in the QSHI phase χ vanishes, consistent with the gapped nature of the insulating state. In contrast, the MI phase exhibits a finite susceptibility that increases as $\chi \sim U$. This paramagnetic behavior suggests the presence of gapless quasiparticles with an emergent Fermi surface [130]. Let us analyze the structure of the gGut solution in this regime. When the MI phase acquires finite magnetization, the spin-imbalance in the impurity orbital is exactly compensated by the decoupled bath state of the impurity model, which in turn is associated with the flat band at the Fermi level in the quasiparticle Hamiltonian. Meanwhile, the other two bath sites, which correspond to the high-energy Hubbard bands, remain unpolarized. Nevertheless, their hybridization with the magnetized impurity is necessarily spin-dependent, leading to $\hat{\mathcal{R}}$ -matrix elements for the Hubbard bands which are different for spin-up and spin-down electrons. In other words, the dispersion of the quasiparticle Hubbard bands develops a spin-dependent renormalization. This occurs in such a way that the spin-up dispersion of the upper Hubbard band exactly matches the spin-down dispersion of the lower Hubbard band,

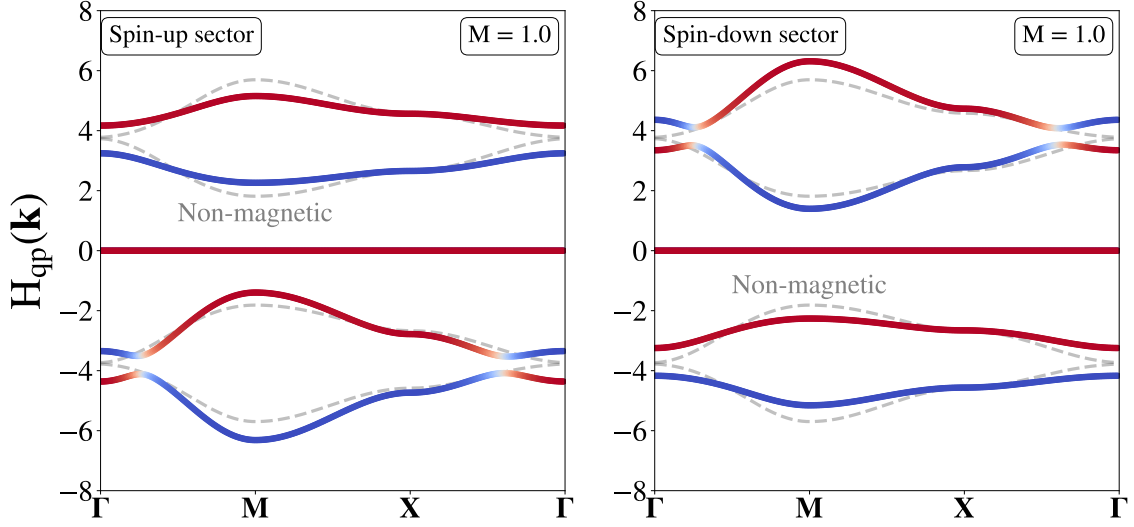


Figure 4.7: Quasiparticle band structure of $H_{\text{qp}}(\mathbf{k})$ showing the renormalization of the Hubbard bands in the presence of a finite magnetization $m = 0.2$ per orbital, for $U = 8.0$ and $M = 1.0$. The color scale indicates the orbital polarization (red for s and blue for p orbital). Gray dashed lines indicate the corresponding band structure in the absence of magnetization. In the spin-up sector, the lower Hubbard bands acquire a non-zero Chern number, while the upper Hubbard bands remain topologically trivial. The opposite occurs in the spin-down sector.

and vice versa.

To understand the origin of this phenomenon, the physical electrons can be considered as composed of multiple fermionic quasiparticles. Indeed, we have already discussed in Sec. 4.1.1 that the renormalization matrix $\hat{\mathcal{R}}$ can be understood as describing how each physical electron is fractionalized into several quasiparticles within the gGut description, as one way of arriving at H_{qp} in Eq. (4.23) is substituting $c_a^\dagger \sim \sum_a \mathcal{R}_{aa}^\dagger f_a^\dagger$. In this sense, the Hubbard quasiparticle bands share the charge density of the physical band, even if its spin is carried in its entirety by the flat quasiparticle band at the Fermi level [130]. At half-filling of the physical electron density, both upper and lower Hubbard bands carry an equal share of the physical electron charge. Yet, when a finite magnetization develops, say along the positive S_z direction, the spin-up physical density exceeds half-filling. Consequently, the spin-up lower Hubbard quasiparticle band becomes its larger contributor, since it is below the Fermi level and thus filled, and sees its $\hat{\mathcal{R}}$ coefficient increased. Meanwhile, the $\hat{\mathcal{R}}$ coefficient of the spin-up upper Hubbard band is decreased. The opposite effect is observed for the spin-down quasiparticle bands, as the spin-down physical density falls below half-filling. In simpler terms, the physical magnetization is not enforced by modifying the occupation of the quasiparticle Hubbard bands, but rather by changing their weights in the physical electron excitation. Furthermore, the above discussion highlights the role—here driven by the magnetization—of this decoupled flat band in determining the dispersion of the Hubbard bands.

In essence, we see that the gGut quasiparticle description of the magnetized MI can be understood in terms of an effective spin-charge separation of the physical electrons, in which the spin component is carried by the decoupled flat quasiparticle band, while the charge component is provided by the quasiparticle Hubbard bands.

Returning to the interplay of topology and magnetism, we specifically leverage the renormalization of the Hubbard band dispersion—induced by spin-dependent $\hat{\mathcal{R}}$ -matrix elements in the presence of finite magnetization—to propose a new mechanism by which the high-energy topological Hubbard bands evolve into spin-selective Chern bands. In this scenario, only one spin species exhibits a non-zero and quantized Chern number. As shown in Fig. 4.7, for a magnetization $m = 0.2$ per orbital, the quasiparticle bands in the spin-up sector are renormalized such that the lower Hubbard bands undergo a band crossing and subsequent gap opening, which can host chiral edge states in OBC, though at finite energy. This follows from the increase of the $\hat{\mathcal{R}}$ coefficient in this band, which accounts for the excess spin-up charge in the physical sites. In contrast, the corresponding upper Hubbard bands in the same spin sector renormalize in the opposite direction and remain topologically trivial. The quasiparticle bands in the spin-down sector exhibit the complementary behavior: the upper Hubbard bands develop a non-trivial topology while the lower bands remain trivial. As a result, the topological structure of the Hubbard bands in this MI phase becomes spin-selective, with a quantized Chern number emerging only for one of the spins. Therefore, the quasiparticle picture in gGut enables simple, single-particle-based descriptions of correlated topology and magnetism, which one can leverage to engineer exotic phases of matter.

4.6 Conclusions

We have shown how the quasiparticle description at the core of the ghost-Gutzwiller (gGut) variational ansatz allows bridging two central pillars of modern condensed matter physics: band-structure topology, rooted in a single-particle description, and strong electronic correlations, which typically undermine such a picture. Working on the paradigmatic interacting BHZ model, we have shown that the quasiparticle Hamiltonian in gGut codifies the topology of the original correlated system, and that it can be used not only for a computationally efficient phase space exploration, but also to model the interplay of topology and correlation with a high-level of interpretability.

A clear demonstration of this interpretability arises in the analysis of the Chern numbers associated with the quasiparticle bands. These quantities offer a transparent and quantitatively accurate interpretation of the Green’s function winding number, currently the state-of-the-art method for characterizing the integrated topology in correlated systems. A major innovation of the gGut framework, however, lies in its ability to capture the topological character of high-energy excitations, such as the Hubbard bands, thereby extending the analysis to energy- and momentum-resolved topological

features. This enables not only a more precise comparison with experimentally accessible ARPES spectra, but also the identification of genuinely nonperturbative features that lie beyond the reach of conventional Density Functional Theory and topological Hamiltonian-based methods. More broadly, we have shown that the gGut formalism promotes a physically grounded interpretation of the Green's function through its quasiparticle structure, offering a step forward in the theoretical understanding of topological phases and their interplay with correlation and magnetism.

CHAPTER 5

Fractionalized Fermi liquids with the ghost-Gutzwiller Ansatz

In this chapter, we discuss how the ghost-Gutzwiller Ansatz can stabilize a fractionalized Fermi liquid (FL) phase in the single-band t - J model. The central methodological ingredients are the extensions of the framework to non-local spin-exchange interactions and to finite temperature. The resulting temperature–doping phase diagram hosts a low-doping FL*, a d -wave superconducting dome, and an overdoped conventional Fermi liquid, thereby reproducing key qualitative features of cuprate phenomenology. This chapter is based on Ref. [48].*

Introduction

The pseudogap normal phase in the underdoped regime is one of the main puzzles surrounding high- T_c cuprate superconductors [160–163]. A longstanding and controversial question, aside from the mechanism behind the pseudogap opening at the anti-nodal points [164], is the topology of the residual Fermi surface at the nodal points. Recent angle-dependent magnetoresistance measurements [165, 166] have finally provided strong and potentially conclusive evidence for the existence of small Fermi pockets that account just for the doping away from half-filling, rather than for the total number of conduction electrons. This clear violation of Luttinger’s theorem [167] is compatible with a pseudogap originating from a Luttinger surface that appears in the Brillouin zone [168–170] upon approaching the half-filled Mott insulator—the very same Green’s-function zeros encountered in Chapter 1. An appealing potential consequence of this scenario is the coexistence of conventional quasiparticles hosted by the Fermi pockets and neutral but spinful ones [59], much in the spirit of Anderson’s spinons in the RVB theory of weakly doped antiferromagnetic Mott insulators [16, 17].

A popular and insightful framework to describe the spin-charge fractionalization of the physical electron [19] is the parton construction, which represents the electron as the product of auxiliary boson and fermion particles, one of which carries the spin and the other the charge [17, 171–178]. In this approach, the quasiparticles at the Fermi pockets, which carry both charge and spin, would appear as bound states of the auxiliary

particles.

Alternatively, one might wish to represent the physical electrons directly in terms of distinct fermionic quasiparticles: one neutral and spinful, and the other bearing both charge and spin. A compelling theoretical realization of this strategy is provided by *fractionalized Fermi liquids* (FL*) [179, 180], whose hallmark is precisely the violation of Luttinger’s theorem. FL* therefore stands out as a natural theoretical target for the pseudogap metal.

The FL* scenario was originally formulated in Kondo-lattice models, where itinerant carriers and localized spins are inherently part of the model. Extending it to single-band models representative of doped Mott insulators is not immediately obvious. A promising attempt in this direction is the recently developed ancilla-qubit construction [181–183], which maps the original single-band problem onto an auxiliary ancilla model with hidden spin layers coupled among themselves and to the physical layer via Kondo exchange terms.

The concept of adding auxiliary fermions beyond the physical electrons to improve the variational description of correlated systems also underpins the ghost-Gutzwiller (gGut) Ansatz introduced in Chapter 4 [122, 125].

In this chapter we demonstrate that the ghost-Gutzwiller approximation can straightforwardly stabilize a FL* phase in the t - J model for cuprate superconductors [184]. A central methodological aspect, to which we devote the first part of the chapter, is the extension of the gGut formalism to non-local spin-exchange interactions, therefore extending the applicability of the method beyond the purely local interactions considered in Chapter 4. Non-local interactions have already been addressed within the standard Gutzwiller approximation [185].

The chapter is organized as follows. In Sec. 5.1 we extend the ghost-Gutzwiller formalism to non-local spin-exchange interactions, deriving the spin-renormalization matrix $\hat{\Theta}(\mathbf{R})$ that carries the exchange coupling over to the auxiliary quasiparticles, in direct analogy with the hopping renormalization of Chapter 4. In Sec. 5.2 we apply the formalism to the single-band t - J model: we introduce a minimal two-bath impurity wavefunction and its associated quasiparticle Hamiltonian, and we identify its two physically relevant limits—the conventional Gutzwiller solution (case A), and the fractionalized solution (case B), which realizes an FL* state where a dispersive spinon coexists with a small, Luttinger-violating hole pocket. In Sec. 5.3 we extend the variational scheme to finite temperature, deriving a computable lower bound for the entropy of the projected density matrix that becomes exact in both the $T \rightarrow 0$ and $T \rightarrow \infty$ limits, and we evaluate it explicitly for the two solutions. Finally, in Sec. 5.4 we present the resulting temperature–doping phase diagram, which hosts a low-doping FL*, a d -wave superconducting dome, and an overdoped conventional Fermi liquid, and we discuss its connection with cuprate phenomenology.

5.1 Extension to non-local spin-spin interactions

In the previous Chapter 4 we have introduced the ghost-Gutzwiller variational wavefunction, $|\Psi_{\text{gGut}}\rangle = \mathcal{P} |\psi_{\text{qp}}\rangle$, and derived the saddle-point equations for a multi-orbital Hamiltonian with purely local interactions, Eq. (4.1). However, the t - J model contains a non-local exchange term. We now discuss how to treat it within the gGut approximation. In order to keep the same notation as in Chapter 4, we write the corresponding Hamiltonian as

$$H = H_{\text{latt}} + \sum_{\mathbf{R}} H_{\text{loc}}(\mathbf{R}) + J \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \vec{S}_{\mathbf{R}} \cdot \vec{S}_{\mathbf{R}'}, \quad (5.1)$$

where H_{latt} is the single-particle hopping, $H_{\text{loc}}(\mathbf{R})$ contains all the local terms at site $\mathbf{R}$, and J is the nearest-neighbour exchange coupling. We restrict the discussion to the single band model, but it can be straightforwardly extended to the multi-orbital case. The physical fermions are collected in the spinor $c_{\mathbf{R}} = (c_{\mathbf{R}\uparrow}, c_{\mathbf{R}\downarrow})^T$, and

$$S_{\mathbf{R}}^{\mu} = c_{\mathbf{R}}^{\dagger} \hat{S}^{\mu} c_{\mathbf{R}}, \quad \hat{S}^{\mu} = \frac{\hat{\sigma}^{\mu}}{2}, \quad \mu = x, y, z, \quad (5.2)$$

with $\hat{\sigma}^{\mu}$ the Pauli matrices. The auxiliary quasiparticle spinors are denoted by $f_{\mathbf{R}a} = (f_{\mathbf{R}a\uparrow}, f_{\mathbf{R}a\downarrow})^T$, where $a = 1, \dots, N_{\text{aux}}$ labels the ghost orbitals introduced in Chapter 4. The non-local exchange expectation value is evaluated with the same Gutzwiller approximation used for the hopping term in Eq. (4.10):

$$\langle \Psi_{\text{gGut}} | \vec{S}_{\mathbf{R}} \cdot \vec{S}_{\mathbf{R}'} | \Psi_{\text{gGut}} \rangle = \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^{\dagger} \vec{S}_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} \mathcal{P}_{\mathbf{R}'}^{\dagger} \vec{S}_{\mathbf{R}'} \mathcal{P}_{\mathbf{R}'} | \psi_{\text{qp}} \rangle. \quad (5.3)$$

The goal is to express the projected spin operator in terms of auxiliary quasiparticle ones. Therefore, in direct analogy with the wave-function renormalization matrix $\hat{\mathcal{R}}(\mathbf{R})$ introduced in Eq. (4.11), we introduce a spin-renormalization matrix $\hat{\Theta}^{\mu}(\mathbf{R})$ through

$$\mathcal{P}_{\mathbf{R}}^{\dagger} S_{\mathbf{R}}^{\mu} \mathcal{P}_{\mathbf{R}} \rightarrow \sum_{a,b=1}^{N_{\text{aux}}} \Theta_{ab}^{\mu}(\mathbf{R}) f_{\mathbf{R}a}^{\dagger} \hat{S}^{\mu} f_{\mathbf{R}b}. \quad (5.4)$$

As in Eq. (4.11), the arrow denotes an equality only at the level of inter-site expectation values; it should not be understood as an operator identity in the full local Hilbert space.

Let us now recall the objects introduced in Chapter 4: the uncorrelated local density matrix

$$(\hat{P}_0(\mathbf{R}))_{nm} = \langle \psi_{\text{qp}} | m, \mathbf{R} \rangle \langle n, \mathbf{R} | \psi_{\text{qp}} \rangle, \quad (5.5)$$

encoding the local probabilities of the quasiparticle state; the matrix $\hat{\Phi}(\mathbf{R})$ of Eq. (4.6), related to the matrix $\hat{\lambda}(\mathbf{R})$, which enters the expression of the local operator $\mathcal{P}_{\mathbf{R}}$, by

$$\hat{\lambda}(\mathbf{R}) = \hat{\Phi}(\mathbf{R}) \sqrt{\hat{P}_0(\mathbf{R})^{-1}}; \quad (5.6)$$

and the local quasiparticle density matrix

$$\Delta_{ab}(\mathbf{R}) = \langle \psi_{\text{qp}} | f_{\mathbf{R}a}^{\dagger} f_{\mathbf{R}b} | \psi_{\text{qp}} \rangle. \quad (5.7)$$

Since $|\psi_{\text{qp}}\rangle$ is a Fock state, its local reduced density matrix is gaussian. Dropping the site label $\mathbf{R}$, and adopting from now on the convention of Chapter 4 that a hat on a fermionic operator denotes its matrix representation in the local auxiliary Fock basis, one can always write

$$\hat{P}_0 = e^{-\beta \hat{H}^0}, \quad \hat{H}^0 = \sum_{ab} h_{ab}^0 \hat{f}_a^\dagger \hat{f}_b - F, \quad (5.8)$$

where $\hat{h}^0 = \hat{h}^{0\dagger}$ is the single-particle entanglement Hamiltonian, the constant F provides the normalization $\text{Tr} \hat{P}_0 = 1$, and β plays the role of an auxiliary inverse temperature. The associated Heisenberg imaginary-time evolution reads

$$\begin{aligned} \hat{f}_a(\tau) &= e^{\hat{H}^0 \tau} \hat{f}_a e^{-\hat{H}^0 \tau} = \hat{f}_a + \tau [\hat{H}^0, \hat{f}_a] + \dots = (e^{-\tau \hat{h}^0} \hat{f})_a \equiv \sum_b \mathcal{U}_{ba}(\tau) \hat{f}_b, \\ \hat{f}_a^\dagger(\tau) &= e^{\hat{H}^0 \tau} \hat{f}_a^\dagger e^{-\hat{H}^0 \tau} = (\hat{f}^\dagger e^{\tau \hat{h}^0})_a \equiv \sum_b \mathcal{U}_{ab}(-\tau) \hat{f}_b^\dagger, \end{aligned} \quad (5.9)$$

where we used $[\hat{H}^0, \hat{f}_a] = -\sum_b h_{ab}^0 \hat{f}_b$. The matrix elements appearing above define the (transpose of the) single-particle propagator

$$\hat{\mathcal{U}}_{\mathbf{R}}(\tau) \equiv \left(e^{-\tau \hat{h}^0(\mathbf{R})} \right)^T. \quad (5.10)$$

In practice $\hat{\mathcal{U}}_{\mathbf{R}}(\tau)$ can be expressed directly in terms of $\hat{\Delta}(\mathbf{R})$, without ever constructing $\hat{h}^0(\mathbf{R})$ explicitly. Using $\hat{P}_0 \hat{f}_b(\beta) = \hat{f}_b \hat{P}_0$, which follows from $\hat{f}_b(\beta) = \hat{P}_0^{-1} \hat{f}_b \hat{P}_0$, the cyclicity of the trace, and $\text{Tr}(\hat{P}_0 \hat{f}_c \hat{f}_a^\dagger) = \delta_{ac} - \Delta_{ac}$, one obtains

$$\begin{aligned} \Delta_{ab} &= \text{Tr}(\hat{P}_0 \hat{f}_a^\dagger \hat{f}_b) = \text{Tr}(\hat{P}_0 \hat{f}_b(\beta) \hat{f}_a^\dagger) \\ &= \sum_c \mathcal{U}_{cb}(\beta) \text{Tr}(\hat{P}_0 \hat{f}_c \hat{f}_a^\dagger) = \mathcal{U}_{ab}(\beta) - \sum_c \Delta_{ac} \mathcal{U}_{cb}(\beta), \end{aligned} \quad (5.11)$$

that is, $\hat{\Delta} = (\mathbb{I} - \hat{\Delta}) \hat{\mathcal{U}}(\beta)$. Inverting this relation yields

$$\hat{\mathcal{U}}_{\mathbf{R}}(\beta) = (\mathbb{I} - \hat{\Delta}(\mathbf{R}))^{-1} \hat{\Delta}(\mathbf{R}), \quad \hat{\mathcal{U}}_{\mathbf{R}}(-\beta) = \hat{\Delta}(\mathbf{R})^{-1} (\mathbb{I} - \hat{\Delta}(\mathbf{R})), \quad (5.12)$$

where the second equality uses $\hat{\mathcal{U}}(-\beta) = \hat{\mathcal{U}}(\beta)^{-1}$. Finally, the last piece we need, before proceeding further in the derivation of the spin-renormalization matrix $\hat{\Theta}^\mu(\mathbf{R})$, is the half-period imaginary-time evolution of the auxiliary fermions

$$\begin{aligned} \sqrt{\hat{P}_0^{-1}} \hat{f}_a \sqrt{\hat{P}_0} &\equiv \hat{f}_a(\beta/2) = \sum_b \mathcal{U}_{ba}(\beta/2) \hat{f}_b, \\ \sqrt{\hat{P}_0^{-1}} \hat{f}_a^\dagger \sqrt{\hat{P}_0} &\equiv \hat{f}_a^\dagger(\beta/2) = \sum_b \mathcal{U}_{ab}(-\beta/2) \hat{f}_b^\dagger. \end{aligned} \quad (5.13)$$

Now, to fix $\hat{\Theta}^\mu(\mathbf{R})$ we follow the same logic as for the renormalization matrix in Chapter 4 [Eq. (4.12)]: the left side of the relation (5.4) is projected onto an auxiliary

spin bilinear $f_{\mathbf{R}a}^\dagger \hat{S}^\mu f_{\mathbf{R}b}$ and evaluated on $|\psi_{\text{qp}}\rangle$. The quantity to be computed is therefore the local expectation value $\langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger c_{\mathbf{R}}^\dagger \hat{S}^\mu c_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} f_{\mathbf{R}a}^\dagger \hat{S}^\mu f_{\mathbf{R}b} | \psi_{\text{qp}} \rangle$. Substituting the parametrization $\hat{\lambda}(\mathbf{R}) = \hat{\Phi}(\mathbf{R}) \sqrt{\hat{P}_0^{-1}(\mathbf{R})}$ of the local projector $\mathcal{P}_{\mathbf{R}}$ [Eq. (4.6)] and using the Gutzwiller factorization of Chapter 4, the expectation value is brought to the trace form of the first equality below, in which the auxiliary operators appear conjugated by $\sqrt{\hat{P}_0(\mathbf{R})}$. Recognizing these conjugated operators as the half-period imaginary-time evolution of Eq. (5.13) then trades the $\sqrt{\hat{P}_0}$ factors for the propagators $\hat{\mathcal{U}}(\pm\beta/2)$, yielding the second equality:

$$\begin{aligned} & \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger c_{\mathbf{R}}^\dagger \hat{S}^\mu c_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} f_{\mathbf{R}a}^\dagger \hat{S}^\mu f_{\mathbf{R}b} | \psi_{\text{qp}} \rangle \\ &= \text{Tr} \left(\hat{\Phi}^\dagger(\mathbf{R}) \hat{c}_{\mathbf{R}}^\dagger \hat{S}^\mu \hat{c}_{\mathbf{R}} \hat{\Phi}(\mathbf{R}) \sqrt{\hat{P}_0^{-1}(\mathbf{R})} \hat{f}_{\mathbf{R}a}^\dagger \hat{S}^\mu \hat{f}_{\mathbf{R}b} \sqrt{\hat{P}_0(\mathbf{R})} \right) \\ &= \sum_{cd} \mathcal{U}_{\mathbf{R},ac}(-\beta/2) \text{Tr} \left(\hat{\Phi}^\dagger(\mathbf{R}) \hat{c}_{\mathbf{R}}^\dagger \hat{S}^\mu \hat{c}_{\mathbf{R}} \hat{\Phi}(\mathbf{R}) \hat{f}_{\mathbf{R}c}^\dagger \hat{S}^\mu \hat{f}_{\mathbf{R}d} \right) \mathcal{U}_{\mathbf{R},db}(\beta/2). \end{aligned} \quad (5.14)$$

The trace appearing in Eq. (5.14) can be rewritten with the embedding wavefunction $|\psi_{\text{imp}}(\mathbf{R})\rangle$ defined in Eq. (4.17). With the same particle-hole convention for the bath states $|\bar{n}\rangle$, one has

$$\begin{aligned} & \langle \psi_{\text{imp}}(\mathbf{R}) | c^\dagger \hat{S}^\mu c f_d \hat{S}^\mu f_c^\dagger | \psi_{\text{imp}}(\mathbf{R}) \rangle \\ &= \sum_{\Gamma n} \sum_{\Gamma' n'} \Phi_{\Gamma n}^*(\mathbf{R}) \Phi_{\Gamma' n'}(\mathbf{R}) e^{-i\phi_\Gamma} e^{i\phi_{\Gamma'}} \langle \bar{n} | \langle \Gamma | c^\dagger \hat{S}^\mu c f_d \hat{S}^\mu f_c^\dagger | \Gamma' \rangle | \bar{n}' \rangle \\ &= \text{Tr} \left(\hat{\Phi}^\dagger(\mathbf{R}) \hat{c}_{\mathbf{R}}^\dagger \hat{S}^\mu \hat{c}_{\mathbf{R}} \hat{\Phi}(\mathbf{R}) \hat{f}_{\mathbf{R}c}^\dagger \hat{S}^\mu \hat{f}_{\mathbf{R}d} \right), \end{aligned} \quad (5.15)$$

where $\phi_\Gamma = \pi n_\Gamma(1 - n_\Gamma)/2$ is the phase already introduced in Eq. (4.17).

In the remainder of this chapter, we will assume that spin $SU(2)$ symmetry is preserved. This implies

$$\begin{aligned} \langle \psi_{\text{qp}} | \mathcal{P}_{\mathbf{R}}^\dagger c_{\mathbf{R}}^\dagger \hat{S}^\mu c_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} f_{\mathbf{R}a}^\dagger \hat{S}^\nu f_{\mathbf{R}b} | \psi_{\text{qp}} \rangle &\propto \delta_{\mu\nu}, \\ \langle \psi_{\text{qp}} | f_{\mathbf{R}a\sigma}^\dagger f_{\mathbf{R}b\sigma'} | \psi_{\text{qp}} \rangle &= \delta_{\sigma\sigma'} \Delta_{ab}(\mathbf{R}). \end{aligned} \quad (5.16)$$

Combining Eqs. (5.4)–(5.16) gives

$$\begin{aligned} & \sum_{cd} \mathcal{U}_{\mathbf{R},ac}(-\beta/2) \langle \psi_{\text{imp}}(\mathbf{R}) | c^\dagger \hat{S}^\mu c f_d \hat{S}^\mu f_c^\dagger | \psi_{\text{imp}}(\mathbf{R}) \rangle \mathcal{U}_{\mathbf{R},db}(\beta/2) \\ &= \frac{1}{2} \sum_{cd} \Theta_{cd}^\mu(\mathbf{R}) \Delta_{cb}(\mathbf{R}) (\delta_{ad} - \Delta_{ad}(\mathbf{R})). \end{aligned} \quad (5.17)$$

The factor $1/2$ comes from the spin trace of $\hat{S}^\mu \hat{S}^\mu$ under the $SU(2)$ -symmetric quasi-particle density matrix.

To recast Eq. (5.17) in closed matrix form, we introduce the matrix

$$T_{ab}^\mu(\mathbf{R}) \equiv \langle \psi_{\text{imp}}(\mathbf{R}) | c^\dagger \hat{S}^\mu c f_a \hat{S}^\mu f_b^\dagger | \psi_{\text{imp}}(\mathbf{R}) \rangle. \quad (5.18)$$

Spin symmetry makes it independent of the spin direction up to a sign, so we denote the common matrix by $\hat{T}(\mathbf{R})$. Indeed, since $\hat{S}^x$ and $\hat{S}^z$ are symmetric while $\hat{S}^y$ is

antisymmetric,

$$\begin{aligned}\langle \psi_{\text{imp}}(\mathbf{R}) | c^\dagger \hat{S}^\mu c f_a \hat{S}^\mu f_b^\dagger | \psi_{\text{imp}}(\mathbf{R}) \rangle &= -T_{ab}(\mathbf{R}), \quad \mu = x, z, \\ \langle \psi_{\text{imp}}(\mathbf{R}) | c^\dagger \hat{S}^y c f_a \hat{S}^y f_b^\dagger | \psi_{\text{imp}}(\mathbf{R}) \rangle &= T_{ab}(\mathbf{R}).\end{aligned}\tag{5.19}$$

Accordingly, $\hat{\Theta}^x(\mathbf{R}) = \hat{\Theta}^z(\mathbf{R}) = -\hat{\Theta}^y(\mathbf{R})$. Choosing $\hat{\Theta}(\mathbf{R}) \equiv \hat{\Theta}^x(\mathbf{R}) = \hat{\Theta}^z(\mathbf{R})$, Eq. (5.17) can be written in matrix form as

$$-\hat{\mathcal{U}}_{\mathbf{R}}(-\beta/2) \hat{T}(\mathbf{R}) \hat{\mathcal{U}}_{\mathbf{R}}(\beta/2) = \frac{1}{2}(\mathbb{I} - \hat{\Delta}(\mathbf{R})) \hat{\Theta}^T(\mathbf{R}) \hat{\Delta}(\mathbf{R}).\tag{5.20}$$

Solving for $\hat{\Theta}(\mathbf{R})$ gives

$$\begin{aligned}\hat{\Theta}^T(\mathbf{R}) &= -2(\mathbb{I} - \hat{\Delta}(\mathbf{R}))^{-1} \hat{\mathcal{U}}_{\mathbf{R}}(-\beta/2) \hat{T}(\mathbf{R}) \hat{\mathcal{U}}_{\mathbf{R}}(\beta/2) \hat{\Delta}(\mathbf{R})^{-1} \\ &= -2\sqrt{(\mathbb{I} - \hat{\Delta}(\mathbf{R}))^{-1} \hat{\Delta}(\mathbf{R})^{-1}} \hat{T}(\mathbf{R}) \sqrt{(\mathbb{I} - \hat{\Delta}(\mathbf{R}))^{-1} \hat{\Delta}(\mathbf{R})^{-1}}.\end{aligned}\tag{5.21}$$

The relative sign between the x, z and y components does not affect the exchange energy, because the non-local term is bilinear in the projected spin operators. The final gGut representation of the exchange interaction is therefore

$$\begin{aligned}\sum_{\mu} \left(\mathcal{P}_{\mathbf{R}}^\dagger c_{\mathbf{R}}^\dagger \hat{S}^\mu c_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} \right) \left(\mathcal{P}_{\mathbf{R}'}^\dagger c_{\mathbf{R}'}^\dagger \hat{S}^\mu c_{\mathbf{R}'} \mathcal{P}_{\mathbf{R}'} \right) \\ \rightarrow \sum_{\mu} \sum_{abcd} \Theta_{ab}(\mathbf{R}) \Theta_{cd}(\mathbf{R}') \left(f_{\mathbf{R}a}^\dagger \hat{S}^\mu f_{\mathbf{R}b} \right) \left(f_{\mathbf{R}'c}^\dagger \hat{S}^\mu f_{\mathbf{R}'d} \right).\end{aligned}\tag{5.22}$$

This equation is the non-local exchange interaction counterpart of the hopping renormalization in Eq. (4.23): the exchange coupling J is transferred to the auxiliary quasiparticle Hamiltonian through the variational matrices $\hat{\Theta}(\mathbf{R})$.

Two remarks close this analysis. First, the renormalized exchange term (5.22) is, by construction, an operator acting purely in the auxiliary quasiparticle space, to be evaluated on the uncorrelated wavefunction $|\psi_{\text{qp}}\rangle$. Since the latter is a Slater determinant or a BCS state, its expectation value follows directly from Wick's theorem, exactly as for the renormalized hopping; the explicit evaluation in the case of a d -wave BCS state is worked out in Appendix A.

Second, the spin-renormalization matrices $\hat{\Theta}(\mathbf{R})$ can be obtained in two equivalent ways. In the following sections we adopt the direct route, projecting the spin operators using the Gutzwiller local operator $\mathcal{P}_{\mathbf{R}}$ explicitly. Equivalently, one could leverage the embedding scheme: the resulting impurity problem would then acquire an additional spin-spin interaction coupling the impurity spin operator to the bath ones, and $\hat{\Theta}(\mathbf{R})$ would be derived from the spin-spin correlation functions, in close analogy to the renormalization factor $\mathcal{R}$. We leave the exploration of this second route to future work.

5.2 Model and variational wavefunction

Equipped with the tools developed in the previous section, we are finally ready to apply the gGut approximation to the t - J model, which is widely used to describe the low-energy physics of cuprate superconductors [19, 186, 187]. The Hamiltonian reads

$$H = - \sum_{\mathbf{R}\mathbf{R}'\sigma} t_{\mathbf{R}\mathbf{R}'} \left(c_{\mathbf{R}\sigma}^\dagger c_{\mathbf{R}'\sigma} + \text{H.c.} \right) + J \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'}, \quad (5.23)$$

with $t_{\mathbf{R}\mathbf{R}'}$ the hopping amplitude between sites $\mathbf{R}$ and $\mathbf{R}'$ of a square lattice, $J > 0$ the exchange coupling between nearest-neighbor spins $\mathbf{S}_{\mathbf{R}} = \sum_{\alpha\beta} c_{\mathbf{R}\alpha}^\dagger \mathbf{S}_{\alpha\beta} c_{\mathbf{R}\beta}$, $\mathbf{S}$ the vector of spin-1/2 matrices, and $c_{\mathbf{R}\sigma}^\dagger$ the creation operator for an electron with spin σ at site $\mathbf{R}$. The local Hilbert space is constrained by the no-double occupancy condition, and we fix the average occupation number per site to $n = 1 - \delta$, with $\delta > 0$.

The variational character of the gGut wavefunction allows us to choose a restricted but physically motivated form of the impurity wavefunction (4.17) encoding the matrix elements of the Gutzwiller local operator $\mathcal{P}_{\mathbf{R}}$ in

$$|\Psi_{\text{gGut}}\rangle = \prod_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} |\psi_{\text{qp}}\rangle, \quad (5.24)$$

thereby simplifying the numerical optimization. Specifically, because of the constraint of no-double occupancy on the impurity, we just retain two bath sites, $a = 1, 2$, where 1 represents a bath pinned at the chemical potential, while bath 2 corresponds to an (almost) empty upper Hubbard band.

We now discuss the most general spin-singlet impurity wavefunction for this two-bath model. As shown below, this minimal two-bath parametrization naturally leads to two distinct ways of accommodating a finite hole density, which are discussed in detail in the following subsections.

5.2.1 Impurity wavefunction and quasiparticle Hamiltonian

We denote the amplitudes of the spin-singlet impurity wavefunction by $\psi(\Gamma; \gamma_1; \gamma_2)$, where $\Gamma \in \{0, \uparrow, \downarrow\}$ labels the physical impurity state, while $\gamma_1, \gamma_2 \in \{0, \uparrow, \downarrow, 2\}$ label the Fock states of bath orbitals 1 and 2. Since the physical site can only be empty or singly occupied, the independent non-vanishing amplitudes can be chosen as

$$\begin{aligned} \psi(\uparrow; \downarrow; 0) &= -\psi(\downarrow; \uparrow; 0) = \frac{\alpha_1}{\sqrt{2}}, \\ \psi(\uparrow; 0; \downarrow) &= -\psi(\downarrow; 0; \uparrow) = \frac{\alpha_2}{\sqrt{2}}, \\ \psi(0; \uparrow; \downarrow) &= -\psi(0; \downarrow; \uparrow) = \frac{\alpha_3}{\sqrt{2}}, \\ \psi(0; 2; 0) &= \alpha_4, \\ \psi(0; 0; 2) &= \alpha_5, \end{aligned} \quad (5.25)$$

with real parameters, which is allowed since the auxiliary impurity model Hamiltonian is real. The wavefunction normalization and the density constraints impose

$$\sum_{i=1}^5 \alpha_i^2 = 1, \quad \alpha_1^2 + \alpha_2^2 = 1 - \delta, \quad \alpha_3^2 + \alpha_4^2 + \alpha_5^2 = \delta. \quad (5.26)$$

Finally, without loss of generality, we choose the bath orbitals to be in their natural basis, which gives the additional condition

$$\langle \psi_{\text{imp}} | f_{1\uparrow}^\dagger f_{2\uparrow} | \psi_{\text{imp}} \rangle = \frac{\alpha_1 \alpha_2}{2} + \frac{\alpha_3(\alpha_4 + \alpha_5)}{\sqrt{2}} = 0. \quad (5.27)$$

Thus the local impurity wavefunction contains two independent variational parameters, in addition to the choice of the uncorrelated quasiparticle state $|\psi_{\text{qp}}\rangle$. A convenient way of solving the constraints is to parametrize the amplitudes as

$$\alpha_3 = \sqrt{\delta} \sin \theta, \quad \alpha_4 = \sqrt{\delta} \cos \theta \cos \phi, \quad \alpha_5 = \sqrt{\delta} \cos \theta \sin \phi. \quad (5.28)$$

Using Eq. (5.27), together with $\alpha_1^2 + \alpha_2^2 = 1 - \delta$, one obtains

$$\begin{aligned} (\alpha_1 + \alpha_2)^2 &= 1 - \delta - \sqrt{2}\delta \sin 2\theta (\cos \phi + \sin \phi), \\ (\alpha_1 - \alpha_2)^2 &= 1 - \delta + \sqrt{2}\delta \sin 2\theta (\cos \phi + \sin \phi). \end{aligned} \quad (5.29)$$

Assuming $\alpha_1^2 > \alpha_2^2$ and $\alpha_1 > 0$, this gives

$$\begin{aligned} \alpha_1 &= \frac{1}{2} \sqrt{1 - \delta - \sqrt{2}\delta \sin 2\theta (\cos \phi + \sin \phi)} + \frac{1}{2} \sqrt{1 - \delta + \sqrt{2}\delta \sin 2\theta (\cos \phi + \sin \phi)}, \\ \alpha_2 &= \frac{1}{2} \sqrt{1 - \delta - \sqrt{2}\delta \sin 2\theta (\cos \phi + \sin \phi)} - \frac{1}{2} \sqrt{1 - \delta + \sqrt{2}\delta \sin 2\theta (\cos \phi + \sin \phi)}. \end{aligned} \quad (5.30)$$

The bath occupations summed over spin in the impurity wavefunction are

$$n_1 = \alpha_1^2 + \alpha_3^2 + 2\alpha_4^2, \quad n_2 = \alpha_2^2 + \alpha_3^2 + 2\alpha_5^2, \quad (5.31)$$

so that $n_1 + n_2 = 1 + \delta$. Since the bath Fock states are related to the auxiliary quasiparticle configurations by a particle-hole transformation, the corresponding local quasiparticle occupations are

$$n_1^{\text{qp}} = 2 - n_1, \quad n_2^{\text{qp}} = 2 - n_2. \quad (5.32)$$

The Gutzwiller constraints imposed on $|\psi_{\text{qp}}\rangle$ are therefore

$$\frac{1}{V} \sum_{\sigma \mathbf{k}} \langle \psi_{\text{qp}} | f_{\mathbf{k}a\sigma}^\dagger f_{\mathbf{k}b\sigma} | \psi_{\text{qp}} \rangle = \delta_{ab} n_a^{\text{qp}}. \quad (5.33)$$

The hopping term renormalization factors are readily obtained, recalling Eqs. (4.11) and (4.20), from

$$\mathcal{R}_a = \frac{\langle \psi_{\text{imp}} | f_{a\sigma}^\dagger c_\sigma | \psi_{\text{imp}} \rangle}{\sqrt{n_{a\sigma}^{\text{qp}}(1 - n_{a\sigma}^{\text{qp}})}}, \quad n_{a\sigma}^{\text{qp}} = \frac{n_a^{\text{qp}}}{2}. \quad (5.34)$$

where

$$\begin{aligned}\langle \psi_{\text{imp}} | f_{1\sigma}^\dagger c_\sigma | \psi_{\text{imp}} \rangle &= \frac{\alpha_1 \alpha_4 + \alpha_2 \alpha_3}{\sqrt{2}}, \\ \langle \psi_{\text{imp}} | f_{2\sigma}^\dagger c_\sigma | \psi_{\text{imp}} \rangle &= \frac{\alpha_2 \alpha_5}{\sqrt{2}} + \frac{\alpha_1 \alpha_3}{2}.\end{aligned}\tag{5.35}$$

We now turn to the spin renormalization factors. The first step is to express the local Gutzwiller projector in the natural basis, where it takes the form

$$\mathcal{P} = \sum_{\Gamma n} \lambda_{\Gamma n} |\Gamma\rangle \langle n|, \quad \lambda_{\Gamma n} = \frac{\Phi_{\Gamma n}}{\sqrt{P_0(n)}}.\tag{5.36}$$

Here Γ labels the physical local states, while n labels the configurations of the local auxiliary Fock space. The quantities $\Phi_{\Gamma n}$ are the amplitudes of the embedded impurity wavefunction introduced in Eq.(5.25), and $P_0(n)$ is the probability of finding the auxiliary configuration n in the uncorrelated quasiparticle state $|\psi_{\text{qp}}\rangle$. Thus the coefficients $\lambda_{\Gamma n}$ are precisely the matrix elements of the local Gutzwiller projector. This representation provides the starting point for identifying the component of the projector that renormalizes the spin operator. Looking at the spin-flip matrix elements, they involve only the components

$$\Phi_{\uparrow,(\uparrow,2)} = \Phi_{\downarrow,(\downarrow,2)} = \frac{\alpha_1}{\sqrt{2}}, \quad \Phi_{\uparrow,(2,\uparrow)} = \Phi_{\downarrow,(2,\downarrow)} = \frac{\alpha_2}{\sqrt{2}},\tag{5.37}$$

where $(\sigma, 2)$ denotes a singly occupied first auxiliary orbital and a doubly occupied second one, while $(2, \sigma)$ denotes the opposite configuration. Therefore the component of the projector acting on the spin operators reads

$$\begin{aligned}\mathcal{P}_{\text{spin}} &= \frac{\alpha_1}{\sqrt{2P_0(\sigma, 2)}} (|\uparrow\rangle \langle \uparrow, 2| + |\downarrow\rangle \langle \downarrow, 2|) \\ &\quad + \frac{\alpha_2}{\sqrt{2P_0(2, \sigma)}} (|\uparrow\rangle \langle 2, \uparrow| + |\downarrow\rangle \langle 2, \downarrow|).\end{aligned}\tag{5.38}$$

The probabilities entering this expression factorize in the uncorrelated quasiparticle state as

$$\begin{aligned}P_0(\sigma, 2) &= \frac{1}{16} n_1^{\text{qp}} (2 - n_1^{\text{qp}}) (n_2^{\text{qp}})^2, \\ P_0(2, \sigma) &= \frac{1}{16} n_2^{\text{qp}} (2 - n_2^{\text{qp}}) (n_1^{\text{qp}})^2.\end{aligned}\tag{5.39}$$

Now, it is sufficient to project $S^+ = |\uparrow\rangle \langle \downarrow|$ explicitly. Since the impurity wavefunction and the quasiparticle state preserve spin $SU(2)$ symmetry, the same renormalization matrix then applies to all components of the spin operator. Applying Eq. (5.38) to S^+ gives

$$\begin{aligned}\mathcal{P}^\dagger S^+ \mathcal{P} &= \frac{\alpha_1^2}{2P_0(\sigma, 2)} |\uparrow, 2\rangle \langle \downarrow, 2| + \frac{\alpha_2^2}{2P_0(2, \sigma)} |2, \uparrow\rangle \langle 2, \downarrow| \\ &\quad + \frac{\alpha_1 \alpha_2}{2\sqrt{P_0(\sigma, 2)P_0(2, \sigma)}} (|\uparrow, 2\rangle \langle 2, \downarrow| + |2, \uparrow\rangle \langle \downarrow, 2|).\end{aligned}\tag{5.40}$$

Using Eq. (5.39), this can be rewritten as

$$\begin{aligned}
 \mathcal{P}^\dagger S^+ \mathcal{P} &= \frac{8\alpha_1^2}{n_1^{\text{qp}}(2 - n_1^{\text{qp}})(n_2^{\text{qp}})^2} |\uparrow, 2\rangle \langle \downarrow, 2| \\
 &+ \frac{8\alpha_2^2}{n_2^{\text{qp}}(2 - n_2^{\text{qp}})(n_1^{\text{qp}})^2} |2, \uparrow\rangle \langle 2, \downarrow| \\
 &+ \frac{8\alpha_1\alpha_2}{n_1^{\text{qp}}n_2^{\text{qp}}\sqrt{n_1^{\text{qp}}n_2^{\text{qp}}(2 - n_1^{\text{qp}})(2 - n_2^{\text{qp}})}} (|\uparrow, 2\rangle \langle 2, \downarrow| + |2, \uparrow\rangle \langle \downarrow, 2|).
 \end{aligned} \tag{5.41}$$

We now express the local Fock state transitions in terms of auxiliary fermions and apply the Gutzwiller approximation. This is not an operator identity: the spin-flip bilinear is kept explicitly, while the density operators on the spectator orbital are replaced by their expectation values in $|\psi_{\text{qp}}\rangle$:

$$\begin{aligned}
 |\uparrow, 2\rangle \langle \downarrow, 2| &= f_{1\uparrow}^\dagger f_{1\downarrow} n_{2\uparrow} n_{2\downarrow} \rightarrow \frac{(n_2^{\text{qp}})^2}{4} f_{1\uparrow}^\dagger f_{1\downarrow}, \\
 |2, \uparrow\rangle \langle 2, \downarrow| &= f_{2\uparrow}^\dagger f_{2\downarrow} n_{1\uparrow} n_{1\downarrow} \rightarrow \frac{(n_1^{\text{qp}})^2}{4} f_{2\uparrow}^\dagger f_{2\downarrow}, \\
 |\uparrow, 2\rangle \langle 2, \downarrow| + |2, \uparrow\rangle \langle \downarrow, 2| &= f_{2\uparrow}^\dagger f_{1\downarrow} n_{1\uparrow} n_{2\downarrow} + f_{1\uparrow}^\dagger f_{2\downarrow} n_{2\uparrow} n_{1\downarrow} \\
 &\rightarrow \frac{n_1^{\text{qp}} n_2^{\text{qp}}}{4} (f_{2\uparrow}^\dagger f_{1\downarrow} + f_{1\uparrow}^\dagger f_{2\downarrow}),
 \end{aligned} \tag{5.42}$$

where $n_{a\sigma}^{\text{qp}} = n_a^{\text{qp}}/2$ has been used. Substituting Eq. (5.42) into Eq. (5.41) gives

$$\begin{aligned}
 \mathcal{P}^\dagger S^+ \mathcal{P} &\rightarrow \frac{2\alpha_1^2}{n_1^{\text{qp}}(2 - n_1^{\text{qp}})} f_{1\uparrow}^\dagger f_{1\downarrow} \\
 &+ \frac{2\alpha_2^2}{n_2^{\text{qp}}(2 - n_2^{\text{qp}})} f_{2\uparrow}^\dagger f_{2\downarrow} \\
 &+ \frac{2\alpha_1\alpha_2}{\sqrt{n_1^{\text{qp}}(2 - n_1^{\text{qp}})n_2^{\text{qp}}(2 - n_2^{\text{qp}})}} (f_{2\uparrow}^\dagger f_{1\downarrow} + f_{1\uparrow}^\dagger f_{2\downarrow}).
 \end{aligned} \tag{5.43}$$

Therefore

$$\mathcal{P}^\dagger S^+ \mathcal{P} \rightarrow \sum_{a,b=1}^2 f_{a\uparrow}^\dagger Q_{ab} f_{b\downarrow}, \tag{5.44}$$

with

$$\begin{aligned}
 Q_{11} &= \frac{2\alpha_1^2}{n_1^{\text{qp}}(2 - n_1^{\text{qp}})}, \\
 Q_{22} &= \frac{2\alpha_2^2}{n_2^{\text{qp}}(2 - n_2^{\text{qp}})}, \\
 Q_{12} &= Q_{21} = \frac{2\alpha_1\alpha_2}{\sqrt{n_1^{\text{qp}}(2 - n_1^{\text{qp}})n_2^{\text{qp}}(2 - n_2^{\text{qp}})}}.
 \end{aligned} \tag{5.45}$$

Gathering all these ingredients together, the variational problem is reduced to minimizing the expectation value of the quasiparticle Hamiltonian

$$H_{\text{qp}} = \sum_{\mathbf{k}\sigma} \sum_{ab}^2 \left(\mathcal{R}_a \mathcal{R}_b \epsilon_{\mathbf{k}} + \lambda_{ab} \right) f_{\mathbf{k}a\sigma}^\dagger f_{\mathbf{k}b\sigma} + J \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \sum_{abcd}^2 Q_{ab} Q_{cd} \mathbf{S}_{\mathbf{R}ab} \cdot \mathbf{S}_{\mathbf{R}'cd}, \tag{5.46}$$

where $\epsilon_{\mathbf{k}}$ is the bare dispersion associated with $t_{\mathbf{R}\mathbf{R}'}$, λ_{ab} the Lagrange multipliers enforcing Eq. (5.33), and $\mathbf{S}_{\mathbf{R}ab} = \sum_{\alpha\beta} f_{\mathbf{R}a\alpha}^\dagger \mathbf{S}_{\alpha\beta} f_{\mathbf{R}b\beta}$.

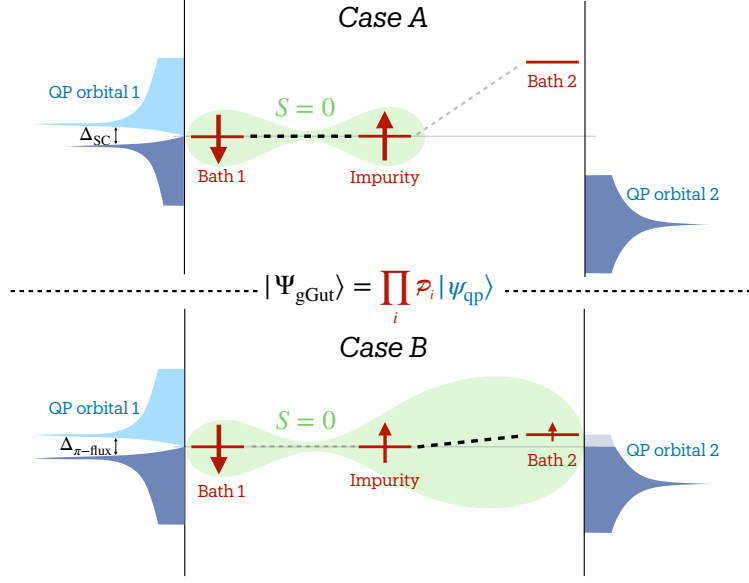


Figure 5.1: Schematic structure of the two-bath ghost-Gutzwiller Ansatz in the two cases considered in the main text. In each panel the central cartoon depicts the impurity model, while the blue lobes on either side are the densities of states of the corresponding auxiliary quasiparticle (QP) bands. Green shading marks a spin singlet ($S = 0$) and a black (gray) dashed line a non-vanishing (vanishing) hybridization. In case A (5.47), the impurity hybridizes and forms a singlet with bath 1, which accommodates the doped charge; the associated auxiliary QP band 1 may develop d -wave quasiparticle pairing Δ_{SC} . Bath 2 stays empty and decoupled. In case B (5.50), bath 1 remains half-filled and unhybridized, but spin-entangled with the impurity, so that QP orbital 1 represents a dispersive spinon (no physical electron spectral weight, $\mathcal{R}_1 = 0$) that may develop π -flux pairing $\Delta_{\pi\text{-flux}}$, while bath 2 is promoted to the Fermi level and carries the doped charge.

5.2.2 Two limiting cases of the impurity wavefunction

Within the minimal two-bath parametrization introduced above, the general impurity wavefunction has two physically relevant limits, which we now discuss. These limits realize two distinct mechanisms for accommodating a finite hole density in the physical orbital, as schematically illustrated in Fig. 5.1.

- A) Similar to the conventional Gutzwiller solution, we can imagine the doped charge to be transferred solely to bath 1. This bath hybridizes with the impurity while the upper Hubbard band, bath 2, remains fully empty and decoupled.
- B) Alternatively, we can consider a scenario where bath 1 remains strictly half-filled, unhybridized with the impurity but strongly spin-entangled with it. In this case the doped charge is transferred to bath 2 which is then promoted to the Fermi level.

Case A) corresponds to the spin-singlet impurity wavefunction

$$|\psi_{\text{imp}}^{\text{A}}\rangle = \frac{\cos \theta}{\sqrt{2}} (|\uparrow; \downarrow, 0\rangle - |\downarrow; \uparrow, 0\rangle) + \sin \theta |0; 2, 0\rangle, \quad (5.47)$$

where $|\gamma_{\text{imp}}; \gamma_1, \gamma_2\rangle$, $\gamma = 0, \uparrow, \downarrow, 2$, are the basis states, and $\cos^2 \theta = 1 - \delta$ is fixed by the physical doping. This wavefunction, corresponding to the general form (5.25) with non-zero amplitudes $\alpha_1 = \cos \theta$ and $\alpha_4 = \sin \theta$, implies $\mathcal{R}_2 = Q_{22} = Q_{12} = 0$ and

$$\mathcal{R}_1 = \sqrt{\frac{2\delta}{1+\delta}}, \quad Q_{11} = \frac{2}{1+\delta}. \quad (5.48)$$

The uncorrelated Fock state $|\psi_{\text{qp}}\rangle$ must be chosen as to minimize the expectation value of the quasiparticle Hamiltonian

$$\begin{aligned} H_{\text{qp}}^{\text{A}} = & -\mathcal{R}_1^2 \sum_{\mathbf{R}\mathbf{R}'\sigma} t_{\mathbf{R}\mathbf{R}'} (f_{\mathbf{R}1\sigma}^\dagger f_{\mathbf{R}'1\sigma} + \text{H.c.}) - \mu \sum_{\mathbf{R}\sigma} f_{\mathbf{R}1\sigma}^\dagger f_{\mathbf{R}1\sigma} \\ & + J Q_{11}^2 \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}1} \cdot \mathbf{S}_{\mathbf{R}'1}, \end{aligned} \quad (5.49)$$

where $\mathbf{S}_{\mathbf{R}1} = \mathbf{S}_{\mathbf{R}11}$ and μ is a Lagrange multiplier that enforces $\langle \sum_{\sigma} f_{\mathbf{R}1\sigma}^\dagger f_{\mathbf{R}1\sigma} \rangle = 1 - \delta$. We observe that Eq. (5.49) is equivalent to the conventional Gutzwiller approach to the t - J model [188]. In fact, the results we are going to show recover those in [171, 188]. In particular, at low doping $|\psi_{\text{qp}}\rangle$ is a BCS wavefunction with d -wave symmetry [171, 188], $\langle f_{1\mathbf{k}\uparrow}^\dagger f_{1-\mathbf{k}\downarrow}^\dagger \rangle = \Delta_{\text{SC}} (\cos k_x - \cos k_y)$, which we denote as SC state; the mean-field decoupling of the exchange on this state is detailed in Appendix A. The order parameter Δ_{SC} , assumed real and positive, is maximum at $\delta = 0$ and decreases monotonically with increasing δ . The physical order parameter, $\Delta = \mathcal{R}_1^2 \Delta_{\text{SC}}$, is instead non-monotonic and vanishes at $\delta = 0$. Above a critical doping, $\Delta_{\text{SC}} = 0$ [171, 188] and $|\psi_{\text{qp}}\rangle$ describes a normal Fermi liquid, which we denote as FL, with a large electron-like Fermi surface that accommodates $1 - \delta$ electrons per site.

Conversely, case B) corresponds to the spin-singlet impurity wavefunction

$$|\psi_{\text{imp}}^{\text{B}}\rangle = \frac{\cos \theta}{\sqrt{2}} (|\uparrow; \downarrow, 0\rangle - |\downarrow; \uparrow, 0\rangle) + \frac{\sin \theta}{\sqrt{2}} (|0; \uparrow, \downarrow\rangle - |0; \downarrow, \uparrow\rangle), \quad (5.50)$$

where, as before, $\cos^2 \theta = 1 - \delta$. Now the non-zero amplitudes in (5.25) are $\alpha_1 = \cos \theta$ and $\alpha_3 = \sin \theta$, which imply $\mathcal{R}_1 = Q_{22} = Q_{12} = 0$ and

$$\mathcal{R}_2 = \sqrt{\frac{1-\delta}{2-\delta}}, \quad Q_{11} = 2(1-\delta). \quad (5.51)$$

The quasiparticle Hamiltonian in this case reads

$$\begin{aligned} H_{\text{qp}}^{\text{B}} = & -\mathcal{R}_2^2 \sum_{\mathbf{R}\mathbf{R}'\sigma} t_{\mathbf{R}\mathbf{R}'} (f_{\mathbf{R}2\sigma}^\dagger f_{\mathbf{R}'2\sigma} + \text{H.c.}) - \mu \sum_{\mathbf{R}\sigma} f_{\mathbf{R}2\sigma}^\dagger f_{\mathbf{R}2\sigma} \\ & + J Q_{11}^2 \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}1} \cdot \mathbf{S}_{\mathbf{R}'1} \equiv H_2^{\text{B}} + H_1^{\text{B}}, \end{aligned} \quad (5.52)$$

where μ enforces $\langle \sum_{\sigma} f_{\mathbf{R}2\sigma}^{\dagger} f_{\mathbf{R}2\sigma} \rangle = 2 - \delta$, while orbital 1 is half-filled. Consequently, the uncorrelated wavefunction factorizes as $|\psi_{\text{qp}}\rangle = |\psi_1\rangle |\psi_2\rangle$ with both $|\psi_1\rangle$ and $|\psi_2\rangle$ Fock states that minimize the expectation value of H_1^{B} and H_2^{B} , respectively, with site-independent local single-particle density matrices. This implies that $|\psi_1\rangle$ is not simply the ground state of the Heisenberg model H_1^{B} , as this is not a Fock state. In reality, the wavefunction $|\psi_1\rangle$ that minimizes the Heisenberg exchange and is consistent with the GA describes a π -flux state [189] or any other equivalent state under the $SU(2)$ gauge symmetry possessed by H_1^{B} [171, 190], such as a d -wave BCS state. For simplicity, we henceforth refer to this state as a π -flux one with order parameter $\Delta_{\pi\text{-flux}} \in \mathbb{R}^+$ that coincides with the above Δ_{SC} at $\delta = 0$. We emphasize that such gauge symmetry simply reflects an invariance property of the Gutzwiller wavefunction (5.24), $\mathcal{P}_{\mathbf{R}} \rightarrow \mathcal{P}_{\mathbf{R}} U_{\mathbf{R}}^{\dagger}$ and $|\psi_{\text{qp}}\rangle \rightarrow \prod_{\mathbf{R}} U_{\mathbf{R}} |\psi_{\text{qp}}\rangle$, with unitary $U_{\mathbf{R}}$, which becomes manifest when the auxiliary fermions have $\mathcal{R} = 0$. The wavefunction $|\psi_2\rangle$ corresponds instead to a conventional metal with a small hole-like Fermi surface that accommodates $2 - \delta$ electrons per site. In other words, $|\psi_{\text{qp}}\rangle = |\psi_1\rangle |\psi_2\rangle$ realizes the FL^* state introduced at the beginning of this chapter: a band of conventional quasiparticles with a Fermi surface that violates Luttinger's theorem, coexisting with a second band of quasiparticles with no physical-electron spectral weight, $\mathcal{R}_1 = 0$. The latter describe fractionalized spinons.

Before further delving into the discussion of the phase diagram obtained for the t - J model within our ghost-Gutzwiller Ansatz, in the following section we discuss how to extend our variational approach to finite temperature, which is necessary to study the stability of the FL^* phase as a function of temperature and doping.

5.3 Variational Ansatz at finite temperature

While the (ghost-)Gutzwiller variational approach was originally formulated at zero temperature, it can be further extended to finite temperature $T \neq 0$ by employing the well-known result that the free energy F associated with the Hamiltonian H satisfies

$$\begin{aligned} F &= \min_{\rho} \left(U(\rho) - T S(\rho) \right) \\ &= \min_{\rho} \left(\text{Tr}(\rho H) + T \text{Tr}(\rho \ln \rho) \right), \end{aligned} \quad (5.53)$$

where ρ spans the space of all density matrices. Restricting the search to a subspace of all possible ρ thus provides an upper bound of the true free-energy. Here, we assume a density matrix [191]

$$\rho_{\text{gGut}} = \prod_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} \rho_{\text{qp}} \mathcal{P}_{\mathbf{R}}^{\dagger} \quad (5.54)$$

where ρ_{qp} is the Boltzmann weight associated with the quasiparticle Hamiltonians (5.49) or (5.52). Following the same spirit of the zero-temperature formulation, we

shall impose the Gutzwiller constraints

$$\begin{aligned}\mathrm{Tr} \left(\rho_{\mathrm{qp}} \mathcal{P}_{\mathbf{R}}^{\dagger} \mathcal{P}_{\mathbf{R}} \right) &= 1 \\ \mathrm{Tr} \left(\rho_{\mathrm{qp}} \mathcal{P}_{\mathbf{R}}^{\dagger} \mathcal{P}_{\mathbf{R}} \mathcal{F}_{\mathbf{R}} \right) &= \mathrm{Tr} \left(\rho_{\mathrm{qp}} \mathcal{F}_{\mathbf{R}} \right)\end{aligned}\tag{5.55}$$

where $\mathcal{F}_{\mathbf{R}}$ is any single-particle operator in the auxiliary space at site $\mathbf{R}$. Following the Gutzwiller approximation, we can thus analytically compute averages over the projected density matrix ρ_{gGut} once the infinite coordination limit is taken. The proof is detailed in [192], hence we shall not repeat it here.

It is now convenient to rewrite the local operator $\mathcal{P}_{\mathbf{R}}$ introducing the components of a temperature dependent variational matrix $\hat{\Phi}(\mathbf{R})$. We define the elements of the temperature dependent positive matrix $\hat{P}_0(\mathbf{R})$ as

$$(\hat{P}_0(\mathbf{R}))_{nm} = \mathrm{Tr} \left(\rho_{\mathrm{qp}} |m, \mathbf{R}\rangle \langle n, \mathbf{R}| \right)\tag{5.56}$$

where $|n, \mathbf{R}\rangle$ are the local Fock states at site $\mathbf{R}$. $\hat{P}_0(\mathbf{R})$ is the single-site reduced density matrix of the auxiliary quasiparticles, obtained by tracing out all other sites from ρ_{qp} . We can then write

$$\mathcal{P}_{\mathbf{R}} = \sum_{\Gamma nm} |\Gamma, \mathbf{R}\rangle \Phi_{\Gamma n}(\mathbf{R}) \left(\hat{P}_0^{-1/2}(\mathbf{R}) \right)_{nm} \langle m, \mathbf{R}| \tag{5.57}$$

where the normalization of the variational density matrix implies that

$$\mathrm{Tr} \left(\mathcal{P}_{\mathbf{R}} \rho_{\mathrm{qp}} \mathcal{P}_{\mathbf{R}}^{\dagger} \right) = \mathrm{Tr} \left(\hat{\Phi}^{\dagger}(\mathbf{R}) \hat{\Phi}(\mathbf{R}) \right) = 1\tag{5.58}$$

As in the conventional Gutzwiller approximation, the internal energy, which in the t - J model does not have any local contribution, can be readily obtained as

$$U(\rho_{\mathrm{qp}}) = \mathrm{Tr}(\rho_{\mathrm{qp}} H_{\mathrm{qp}})\tag{5.59}$$

where the expectation value of the auxiliary quasiparticle Hamiltonian on the uncorrelated state $|\psi_{\mathrm{qp}}\rangle$ has been replaced by the thermal average over the quasiparticle density matrix ρ_{qp} .

To get the free energy, which is the relevant quantity to minimize at finite temperature, we also need to compute the entropy of the variational density matrix. Since a closed expression for $S(\rho_{\mathrm{gGut}})$ cannot be found within the GA, we use a lower bound that extends the one in [191] and becomes exact in both $T = 0$ and $T \rightarrow \infty$ limits, derived in the following and given by Eq. (5.78).

5.3.1 A lower bound for the entropy

We define $\mathcal{Q}_{\mathbf{R}}$, not to be confused with the spin renormalization matrix Q_{ab} , as

$$\mathcal{Q}_{\mathbf{R}} = \mathcal{P}_{\mathbf{R}}^{\dagger} \mathcal{P}_{\mathbf{R}}, \quad \mathcal{P}_{\mathbf{R}} = U_{\mathbf{R}} \sqrt{\mathcal{Q}_{\mathbf{R}}}, \quad \mathcal{P}_{\mathbf{R}}^{\dagger} = \sqrt{\mathcal{Q}_{\mathbf{R}}} U_{\mathbf{R}}^{\dagger}\tag{5.60}$$

with unitaries $U_{\mathbf{R}}$, so that

$$\mathcal{Q} = \prod_{\mathbf{R}} \mathcal{Q}_{\mathbf{R}}, \quad \mathcal{P} = U \sqrt{\mathcal{Q}}, \quad \mathcal{P}^\dagger = \sqrt{\mathcal{Q}} U^\dagger. \quad (5.61)$$

It follows that

$$\begin{aligned} S(\rho_{\text{gGut}}) &= -\text{Tr} \left(U \sqrt{\mathcal{Q}} \rho_{\text{qp}} \sqrt{\mathcal{Q}} U^\dagger \ln(U \sqrt{\mathcal{Q}} \rho_{\text{qp}} \sqrt{\mathcal{Q}} U^\dagger) \right) \\ &= -\text{Tr} \left(\sqrt{\mathcal{Q}} \rho_{\text{qp}} \sqrt{\mathcal{Q}} \ln(\sqrt{\mathcal{Q}} \rho_{\text{qp}} \sqrt{\mathcal{Q}}) \right). \end{aligned} \quad (5.62)$$

A first lower bound for the entropy $S(\rho_{\text{gGut}})$ follows from the Golden-Thompson-type trace inequality

$$\text{Tr}(X \ln X) \leq \text{Tr}(X \ln Y) + \text{Tr}(X \ln(XY^{-1})), \quad (5.63)$$

which implies, for $X = \mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{1/2}$ and $Y = \mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{-1/2}$, and using the Gutzwiller constraints with $\ln \rho_{\text{qp}}$ a one-body operator, that

$$\begin{aligned} S(\rho_{\text{gGut}}) &\geq -\text{Tr}(\rho_{\text{qp}} \mathcal{Q} \ln \rho_{\text{qp}}) - \text{Tr}(\mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{1/2} \ln \mathcal{Q}) \\ &= S(\rho_{\text{qp}}) - \sum_{\mathbf{R}} \text{Tr} \left(\sqrt{\mathcal{Q}_{\mathbf{R}}} \hat{P}_0(\mathbf{R}) \sqrt{\mathcal{Q}_{\mathbf{R}}} \ln \mathcal{Q}_{\mathbf{R}} \right) \\ &= S(\rho_{\text{qp}}) - \sum_{\mathbf{R}} \text{Tr}(\mathcal{Q}_{\mathbf{R}} \hat{P}_0(\mathbf{R}) \ln \mathcal{Q}_{\mathbf{R}}) \\ &= S(\rho_{\text{qp}}) - \sum_{\mathbf{R}} \text{Tr} \left(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\Phi}(\mathbf{R}) \ln(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\Phi}(\mathbf{R}) \hat{P}_0(\mathbf{R})^{-1}) \right). \end{aligned} \quad (5.64)$$

where in the last equality we used the definition of $\mathcal{P}_{\mathbf{R}}$ in terms of $\hat{\Phi}(\mathbf{R})$ and $\hat{P}_0(\mathbf{R})$ (see Eq. (5.57)).

However, this is a very poor bound, since its right-hand side can become negative. To find a better lower bound, we employ the following inequality [193]

$$\text{Tr}(X \ln X) \leq \text{Tr}(X \ln Y) + \frac{1}{p} \text{Tr}(X \ln(X^p Y^{-p})), \quad (5.65)$$

which reduces to the previous one for $p = 1$, while we obtain a tighter lower bound on $S(\rho_{\text{gGut}})$ for $p < 1$ that becomes an equality for $p \rightarrow 0$:

$$\begin{aligned} S(\rho_{\text{gGut}}) - S(\rho_{\text{qp}}) &\geq -\frac{1}{p} \text{Tr} \left(\mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{1/2} \ln \left((\mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{1/2})^p (\mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{-1/2})^{-p} \right) \right) \\ &\equiv -D_p(\rho_{\text{qp}}, \mathcal{Q}). \end{aligned} \quad (5.66)$$

We emphasize that this lower bound becomes tighter as p decreases from 1 to 0 [193]. Furthermore, since we can reasonably expect that $S(\rho_{\text{gGut}}) < S(\rho_{\text{qp}})$ (the local operator $\mathcal{P}$ acts as a filter on the auxiliary quasiparticle density matrix ρ_{qp}) and $D_p(\rho_{\text{qp}}, \mathcal{Q}) > 0$, we can write

$$D_p(\rho_{\text{qp}}, \mathcal{Q}) := S(\rho_{\text{qp}}) W_p(\rho_{\text{qp}}, \mathcal{Q}), \quad (5.67)$$

with $W_p(\rho_{\text{qp}}, \mathcal{Q}) > 0$. Thus,

$$S(\rho_{\text{gGut}}) \geq S(\rho_{\text{qp}}) (1 - W_p(\rho_{\text{qp}}, \mathcal{Q})), \quad p \in [0, 1]. \quad (5.68)$$

For $T \rightarrow \infty$, $\rho_{\text{qp}} \rightarrow 1/d$, where d is the dimension of the local auxiliary Hilbert space, so that

$$\mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{1/2} \rightarrow \mathcal{Q}/d, \quad \mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{-1/2} \rightarrow \mathbb{1}/d. \quad (5.69)$$

The argument of the logarithm in D_p then simplifies to

$$(\mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{1/2})^p (\mathcal{Q}^{1/2} \rho_{\text{qp}} \mathcal{Q}^{-1/2})^{-p} \rightarrow \left(\frac{\mathcal{Q}}{d}\right)^p \left(\frac{\mathbb{1}}{d}\right)^{-p} = \mathcal{Q}^p, \quad (5.70)$$

so that

$$D_p(\rho_{\text{qp}}, \mathcal{Q}) \rightarrow \frac{1}{d} \text{Tr}(\mathcal{Q} \ln \mathcal{Q}), \quad (5.71)$$

which is independent of p , and hence so is $W_p(\rho_{\text{qp}}, \mathcal{Q})$. Moreover, $W_p(\rho_{\text{qp}}, \mathcal{Q})$ decreases monotonically with decreasing p from 1 to 0 [193], which implies

$$0 < W_0(\rho_{\text{qp}}, \mathcal{Q}) \equiv \frac{S(\rho_{\text{qp}}) - S(\rho_{\text{gGut}})}{S(\rho_{\text{qp}})} \leq W_p(\rho_{\text{qp}}, \mathcal{Q}) \leq W_1(\rho_{\text{qp}}, \mathcal{Q}). \quad (5.72)$$

On the other hand, since $S(\rho_{\text{qp}})$ increases with T , being maximum and equal to S_∞ at $T \rightarrow \infty$,

$$W_1(\rho_{\text{qp}}, \mathcal{Q}) = \frac{D_1(\rho_{\text{qp}}, \mathcal{Q})}{S(\rho_{\text{qp}})} \geq \frac{D_1(\rho_{\text{qp}}, \mathcal{Q})}{S_\infty}. \quad (5.73)$$

We now wish to demonstrate that there exists a p with $0 < p < 1$ such that

$$W_0(\rho_{\text{qp}}, \mathcal{Q}) \leq W_p(\rho_{\text{qp}}, \mathcal{Q}) = \frac{D_p(\rho_{\text{qp}}, \mathcal{Q})}{S(\rho_{\text{qp}})} \leq \frac{D_1(\rho_{\text{qp}}, \mathcal{Q})}{S_\infty} \leq W_1(\rho_{\text{qp}}, \mathcal{Q}). \quad (5.74)$$

We assume that $S(\rho_{\text{qp}}) \rightarrow 0$ for $T \rightarrow 0$, which implies $S(\rho_{\text{gGut}}) \rightarrow 0$ as well. If both vanish in the same way, as expected when ρ_{qp} and ρ_{gGut} describe the same low-energy physics, then $W_0(\rho_{\text{qp}}, \mathcal{Q}) \rightarrow 0$, and the chain of inequalities

$$W_0(\rho_{\text{qp}}, \mathcal{Q}) \equiv 0 \leq W_p(\rho_{\text{qp}}, \mathcal{Q}) \leq \frac{D_1(\rho_{\text{qp}}, \mathcal{Q})}{S_\infty} \leq W_1(\rho_{\text{qp}}, \mathcal{Q}), \quad (5.75)$$

holds strictly for p sufficiently close to 0. Equation (5.75) remains valid even if

$$\lim_{T \rightarrow 0} \frac{S(\rho_{\text{qp}}) - S(\rho_{\text{gGut}})}{S(\rho_{\text{qp}})} = C > 0, \quad (5.76)$$

provided $C \leq D_1(\rho_{\text{qp}}, \mathcal{Q})/S_\infty$ for all T .

Let us summarize what the chain of inequalities (5.75) establishes. The exact entropy deficit of the variational state is encoded in $W_0(\rho_{\text{qp}}, \mathcal{Q}) = [S(\rho_{\text{qp}}) - S(\rho_{\text{gGut}})]/S(\rho_{\text{qp}})$, which is not accessible within the GA. Equation (5.75) shows that the single quantity

$$\frac{D_1(\rho_{\text{qp}}, \mathcal{Q})}{S_\infty} \quad (5.77)$$

is bounded from below and above by the exact deficit W_0 and the loose estimate W_1 respectively, i.e. $W_0 \leq D_1(\rho_{\text{qp}}, \mathcal{Q})/S_\infty \leq W_1$. Because it lies *above* W_0 , replacing the true deficit by D_1/S_∞ can only underestimate the entropy, so it provides a lower

bound. Crucially, D_1/S_∞ depends only on the saddle-point objects $\mathcal{Q}$ and ρ_{qp} and on the dimension d of the local auxiliary Hilbert space, so it is fully computable within the GA at no extra cost.

Identifying the infinite-temperature entropy with $S_\infty = N \ln d$ and using $D_1(\rho_{\text{qp}}, \mathcal{Q}) = \text{Tr}(\rho_{\text{qp}} \mathcal{Q} \ln \mathcal{Q})$, we therefore arrive at

$$S(\rho_{\text{gGut}}) \geq S(\rho_{\text{qp}}) \left(1 - \frac{\text{Tr}(\rho_{\text{qp}} \mathcal{Q} \ln \mathcal{Q})}{N \ln d} \right), \quad (5.78)$$

which is the lower bound on the entropy that we shall adopt in the finite-temperature calculations. Inserted into $F \leq U(\rho_{\text{gGut}}) - T S(\rho_{\text{gGut}})$, it preserves the upper bound on the free energy and hence the variational character of the finite-temperature ghost-Gutzwiller scheme.

5.3.2 Explicit evaluation of the entropy bound in the two limiting cases

We now explicitly evaluate the two ingredients entering the entropy bound, the distortion term

$$\begin{aligned} D_1(\rho_{\text{qp}}, \mathcal{Q}) &= \text{Tr}(\rho_{\text{qp}} \mathcal{Q} \ln \mathcal{Q}) \\ &= \sum_{\mathbf{R}} \text{Tr}(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\Phi}(\mathbf{R}) \ln(\hat{\Phi}^\dagger(\mathbf{R}) \hat{\Phi}(\mathbf{R}) \hat{P}_0(\mathbf{R})^{-1})) \end{aligned} \quad (5.79)$$

and the infinite temperature limit of the quasiparticle entropy $S_\infty = \ln d$, for the two limiting cases discussed above. Both quantities are extensive, and we quote them per site; the estimate involves only their intensive ratio. In both cases we work in the local Fock basis $\{0, \uparrow, \downarrow, 2\}$ of the auxiliary orbitals, and we use the impurity amplitudes of Eqs. (5.47)–(5.50) together with the auxiliary occupations quoted above.

Conventional Gutzwiller solution (case A)

In this case orbital 2 is doubly occupied and factorizes out, leaving the four-dimensional local space of orbital 1, whose reduced density matrix and variational matrix are both diagonal,

$$\begin{aligned} \hat{P}_0 &= \frac{1}{4} \text{diag}((1 + \delta)^2, 1 - \delta^2, 1 - \delta^2, (1 - \delta)^2), \\ \hat{\Phi}^\dagger \hat{\Phi} &= \text{diag}\left(\delta, \frac{1 - \delta}{2}, \frac{1 - \delta}{2}, 0\right). \end{aligned} \quad (5.80)$$

The distortion term and the infinite-temperature entropy per site thus read

$$\begin{aligned} \frac{D_1}{N} &= \delta \ln \frac{4\delta}{(1 + \delta)^2} - (1 - \delta) \ln \frac{1 + \delta}{2}, \\ \frac{S_\infty}{N} &= -(1 - \delta) \ln \frac{1 - \delta}{2} - (1 + \delta) \ln \frac{1 + \delta}{2}, \end{aligned} \quad (5.81)$$

where S_∞/N is the entropy per site of $2N$ auxiliary spin-orbitals hosting $(1 - \delta)N$ fermions, obtained from the binomial count in the Stirling limit.

Fractionalized FL^* solution (case B)

Now both orbitals are active: orbital 1 is half-filled and orbital 2 hosts $2 - \delta$ electrons. In the four-dimensional subspace $\{(\uparrow, 2), (\downarrow, 2), (\uparrow, \downarrow), (\downarrow, \uparrow)\}$ the variational matrix acquires a non-diagonal singlet block,

$$\hat{\Phi}^\dagger \hat{\Phi} = \frac{1-\delta}{2} (|\uparrow, 2\rangle \langle \uparrow, 2| + |\downarrow, 2\rangle \langle \downarrow, 2|) + \frac{\delta}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}_{\{(\uparrow, \downarrow), (\downarrow, \uparrow)\}}, \quad (5.82)$$

while the reduced density matrix stays diagonal, with entries

$$\begin{aligned} \langle \uparrow, 2 | \hat{P}_0 | \uparrow, 2 \rangle &= \langle \downarrow, 2 | \hat{P}_0 | \downarrow, 2 \rangle = n_{1\sigma}^{\text{qp}}(1 - n_{1\sigma}^{\text{qp}})(n_{2\sigma}^{\text{qp}})^2 = (2 - \delta)^2/16, \\ \langle \uparrow, \downarrow | \hat{P}_0 | \uparrow, \downarrow \rangle &= \langle \downarrow, \uparrow | \hat{P}_0 | \downarrow, \uparrow \rangle = n_{1\sigma}^{\text{qp}}(1 - n_{1\sigma}^{\text{qp}})n_{2\sigma}^{\text{qp}}(1 - n_{2\sigma}^{\text{qp}}) = (2 - \delta)\delta/16 \end{aligned} \quad (5.83)$$

Since $\hat{P}_0$ is proportional to the identity within the singlet block of $\hat{\Phi}^\dagger \hat{\Phi}$, that block contributes only through the non-zero eigenvalue δ of $\hat{\Phi}^\dagger \hat{\Phi}$, giving

$$\begin{aligned} \frac{D_1}{N} &= (1 - \delta) \ln \frac{2(1 - \delta)}{(1 - \delta/2)^2} + \delta \ln \frac{8}{1 - \delta/2}, \\ \frac{S_\infty}{N} &= \ln 4 - (2 - \delta) \ln \frac{2 - \delta}{2} - \delta \ln \frac{\delta}{2}, \end{aligned} \quad (5.84)$$

the latter being the sum of the entropies per site of a half-filled orbital and an orbital at filling $2 - \delta$.

High-temperature consistency

We can explicitly verify that for both solutions the estimate saturates correctly as $T \rightarrow \infty$: subtracting the distortion term from S_∞ recovers the exact infinite-temperature entropy of the t - J model at doping δ ,

$$\frac{S_\infty - D_1}{N} = -\delta \ln \delta - (1 - \delta) \ln \frac{1 - \delta}{2}, \quad (5.85)$$

i.e. the configurational entropy of δN empty and $(1 - \delta)N$ singly-occupied sites. The identity holds for case A and case B alike, confirming that the D_1/S_∞ estimate is exact at high-temperature in both the conventional and the fractionalized phase.

5.4 Temperature–doping phase diagram

We are now ready to discuss the variational temperature-doping phase diagram of the t - J model within our ghost-Gutzwiller Ansatz. The parameters in Eq. (5.23) are chosen to represent the one-band description of cuprates [186, 187]: Heisenberg coupling $J/t = 0.4$, nearest-neighbor hopping $t = 1$, and next-nearest-neighbor hopping $t'/t = -0.4$.

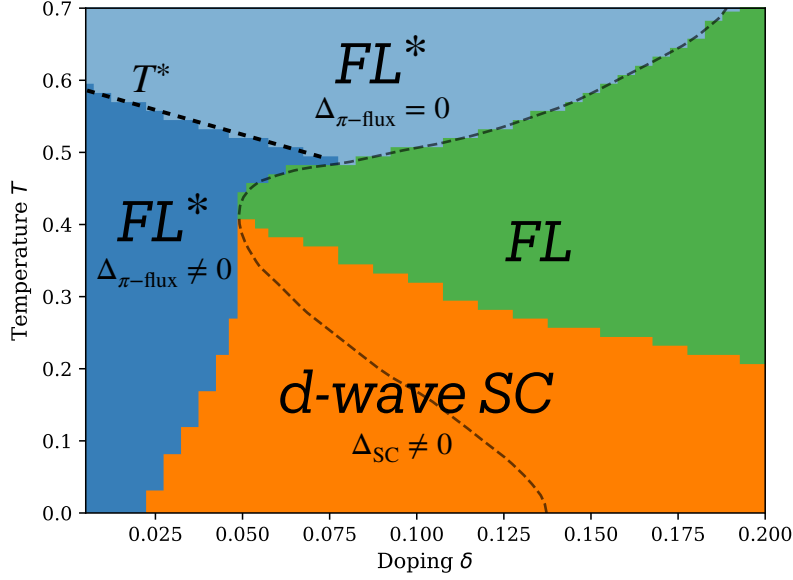


Figure 5.2: Temperature–doping phase diagram of the t - J model ($J/t = 0.4$, $t'/t = -0.4$, $t = 1$) within the ghost-Gutzwiller Ansatz. At low doping the normal state is a fractionalized Fermi liquid (FL^*) with a small, hole-like Fermi surface accounting just for the doped holes; the overdoped normal state is a conventional FL with a large, electron-like Fermi surface satisfying Luttinger’s count. The gray dashed line marks the boundary between the two metallic states preventing superconductivity. Within the FL^* region, the black dashed line is the spinon pairing scale T^* , below which the π -flux order parameter $\Delta_{\pi\text{-flux}}$ is finite. When superconductivity is allowed, a d -wave superconducting dome ($\Delta_{SC} \neq 0$) intrudes between the two metallic regimes.

The resulting phase diagram is shown in Fig. 5.2. At low doping, the optimal impurity wavefunction is of type B (5.50) and yields a FL^* phase. The π -flux order parameter $\Delta_{\pi\text{-flux}}$ is finite below $T^* \propto Q_{11}^2 J \sim (1 - \delta)^2$ and zero above. It is thus tempting to associate T^* with the pseudogap temperature in cuprates. If superconductivity is prevented, the FL^* transitions above a critical doping into a conventional FL state characterized by the A-type impurity wavefunction (5.47). This is shown by the gray dashed line in Fig. 5.2 and corresponds to a reconstruction of the Fermi surface from hole-like to electron-like. Allowing for superconductivity, implicitly assuming an inter-layer hopping that stabilizes phase coherence, results in the SC dome depicted in Fig. 5.2, which is again associated with the impurity wavefunction (5.47). In the slave-boson mean-field theory of the t - J model [171], the superconducting dome emerges from the interplay of two distinct temperatures: the slave-boson condensation temperature, which is zero at $\delta = 0$ and rises with doping, and the temperature at which the quasiparticle d -wave order parameter Δ_{SC} vanishes, which decreases monotonically with increasing δ . In our calculation, the dome is a result of the competition between the larger internal energy of the SC phase and the larger entropy of the FL^* and FL states, since both have Fermi surfaces.

The transition lines between the SC/FL and the FL^* phases arise from the two distinct

impurity wavefunctions (5.47) and (5.50), respectively. Consequently, these transitions mark the crossing of their respective free energies and are therefore first-order. We anticipate that optimizing the variational free-energy with the most general impurity wavefunction (5.25) incorporating (5.47) and (5.50) as special cases would modify the transition lines and the precise shape of the phase diagram, but not its overall features. This more involved calculation, although valuable, exceeds the scope of this chapter, which is to demonstrate the potential of the ghost Gutzwiller approximation to capture exotic phases such as FL^* at extremely low computational cost.

5.5 Conclusions

We have demonstrated that the ghost-Gutzwiller approximation applied to the single-band t - J model provides a straightforward variational route to a fractionalized Fermi liquid (FL^*), characterized by neutral yet spinful quasiparticles coexisting with conventional ones that form hole-like Fermi pockets whose volume is set solely by the doping away from half-filling. The violation of Luttinger's theorem that defines the FL^* is thus realized within a purely variational, mean-field-level calculation, and is intimately tied to the Green's function zeros that accompany the approach to the half-filled Mott insulator, encountered already in Chapter 1.

Despite its minimal structure, the Ansatz successfully reproduces the essential qualitative features of the cuprate phase diagram: a low-doping FL^* metal, a d -wave superconducting dome, and an overdoped conventional Fermi liquid with a large Fermi surface. In the FL^* regime, the spinons arrange into a π -flux phase, which is gauge equivalent to a d -wave condensate, below a temperature scale T^* associated with the onset of pseudogap behavior. This does not, however, directly produce a physical superconducting order parameter. Superconductivity emerges only when the paired spinons acquire physical electron spectral weight through the Gutzwiller projection.

We emphasize that stabilizing the FL^* phase relies on the nonlocal character of the spin-exchange interaction, which endows the self-energy with a genuine momentum dependence that a purely local interaction would not produce within the Gutzwiller approximation. Accessing this regime required generalizing the ghost-Gutzwiller framework, originally formulated for purely local interactions, to account for non-local spin-exchange terms. This is, however, not equivalent to a conventional mean-field decoupling of the exchange term: in the present case, the interaction is first dressed by the Gutzwiller operator $\mathcal{P}$, which renormalizes the effective quasiparticle dynamics and may also induce a frequency-dependent self-energy. We mention that preliminary calculations suggest that an analogous FL^* solution can persist as a metastable state also in the doped single-band Hubbard model deep in the Mott regime, which we leave for future work.

In a broader context, the flexibility and low cost of the ghost-Gutzwiller Ansatz render it a promising tool for investigating FL^* and related unexplored phases in multi-orbital

models of correlated materials. This approach may offer a complementary variational perspective to more computationally expensive methods, such as cluster extensions of dynamical mean-field theory [32, 194, 195] and variational Monte Carlo based on projected parton wave functions [196–198], which can study similar fractionalized regimes but at significantly higher computational expense. This comparison may aid in clarifying, for instance, the microscopic origin of experimentally observed insulators with gapless neutral excitations despite the finite charge gap [28, 78, 199].

A Mean-field decoupling of the spin-spin exchange on a d -wave BCS state

In this appendix we detail the mean-field decoupling of the nearest-neighbour spin exchange and the evaluation of its expectation value on a BCS wavefunction with d -wave symmetry. This is precisely the calculation needed to evaluate the renormalized exchange term of the quasiparticle Hamiltonian (5.46) on the uncorrelated state $|\psi_{\text{qp}}\rangle$ when the latter is a d -wave superconductor, as in case A [Eq. (5.49)]. In both limiting cases (5.47)–(5.50) only orbital 1 carries the exchange, so throughout this appendix we suppress the orbital index and write $f \equiv f_1$, and we denote by $\tilde{J} \equiv J Q_{11}^2$ the renormalized coupling. The auxiliary quasiparticle spin is $\mathbf{S}_{\mathbf{R}} = \sum_{\alpha\beta} f_{\mathbf{R}\alpha}^\dagger \mathbf{S}_{\alpha\beta} f_{\mathbf{R}\beta}$. Fourier transforming, the nearest-neighbour exchange on the square lattice ($2V$ bonds) becomes

$$\tilde{J} \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'} = \frac{\tilde{J}}{V} \sum_{\mathbf{q}} \gamma(\mathbf{q}) \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}}, \quad \gamma(\mathbf{q}) = \cos q_x + \cos q_y, \quad (5.86)$$

which, splitting the spin product into its longitudinal and transverse parts and expressing it through the quasiparticle operators, reads

$$\begin{aligned} \tilde{J} \sum_{\langle \mathbf{R}\mathbf{R}' \rangle} \mathbf{S}_{\mathbf{R}} \cdot \mathbf{S}_{\mathbf{R}'} &= \frac{\tilde{J}}{4V} \sum_{\mathbf{q}\mathbf{k}\mathbf{p}} \gamma(\mathbf{q}) (f_{\mathbf{k}\uparrow}^\dagger f_{\mathbf{k}+\mathbf{q}\uparrow} - f_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{k}+\mathbf{q}\downarrow}) (f_{\mathbf{p}+\mathbf{q}\uparrow}^\dagger f_{\mathbf{p}\uparrow} - f_{\mathbf{p}+\mathbf{q}\downarrow}^\dagger f_{\mathbf{p}\downarrow}) \\ &\quad + \frac{\tilde{J}}{2V} \sum_{\mathbf{q}\mathbf{k}\mathbf{p}} \gamma(\mathbf{q}) (f_{\mathbf{k}\uparrow}^\dagger f_{\mathbf{k}+\mathbf{q}\downarrow} f_{\mathbf{p}+\mathbf{q}\downarrow}^\dagger f_{\mathbf{p}\uparrow} + f_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{k}+\mathbf{q}\uparrow} f_{\mathbf{p}+\mathbf{q}\uparrow}^\dagger f_{\mathbf{p}\downarrow}). \end{aligned} \quad (5.87)$$

We evaluate its expectation value on the single-band BCS wavefunction

$$|\psi_{\text{qp}}\rangle = \prod_{\mathbf{k}} (\sin \theta_{\mathbf{k}} + \cos \theta_{\mathbf{k}} f_{\mathbf{k}\uparrow}^\dagger f_{-\mathbf{k}\downarrow}^\dagger) |0\rangle \equiv \prod_{\mathbf{k}} |\psi_{\mathbf{k}}\rangle, \quad (5.88)$$

whose only non-vanishing normal and anomalous averages are

$$\begin{aligned} 2n_{\mathbf{k}} - 1 &\equiv \langle \psi_{\mathbf{k}} | (n_{\mathbf{k}\uparrow} + n_{-\mathbf{k}\downarrow}) | \psi_{\mathbf{k}} \rangle = \cos 2\theta_{\mathbf{k}}, \\ \Delta_{\mathbf{k}} &\equiv \langle \psi_{\mathbf{k}} | f_{\mathbf{k}\uparrow}^\dagger f_{-\mathbf{k}\downarrow}^\dagger | \psi_{\mathbf{k}} \rangle = \frac{1}{2} \sin 2\theta_{\mathbf{k}}. \end{aligned} \quad (5.89)$$

Fixing the orbital filling to $1 - \delta$ imposes

$$1 - \delta = \frac{1}{V} \sum_{\mathbf{k}} \langle \psi_{\mathbf{k}} | (n_{\mathbf{k}\uparrow} + n_{-\mathbf{k}\downarrow}) | \psi_{\mathbf{k}} \rangle = 1 + \frac{1}{V} \sum_{\mathbf{k}} \cos 2\theta_{\mathbf{k}}, \quad (5.90)$$

while the hopping energy per site reads

$$E_t = -\frac{2t}{V} \mathcal{R}_1^2 \sum_{\mathbf{k}} (\cos k_x + \cos k_y) \cos 2\theta_{\mathbf{k}}. \quad (5.91)$$

We evaluate the exchange energy by applying Wick's theorem to (5.87), which generates two families of contractions.

Normal contractions. Contracting each fermion bilinear separately gives the Fock (exchange) channel, in which the pairing of $f_{\mathbf{k}+\mathbf{q}}$ with $f_{\mathbf{p}+\mathbf{q}}^\dagger$ enforces $\mathbf{k} = \mathbf{p}$, and relabelling the momentum transfer as $\mathbf{k} - \mathbf{p}$ leaves

$$\begin{aligned} E_J^N &= \frac{\tilde{J}}{4V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) \left(\langle f_{\mathbf{k}\uparrow}^\dagger f_{\mathbf{k}\uparrow} \rangle \langle f_{\mathbf{p}\uparrow} f_{\mathbf{p}\uparrow}^\dagger \rangle + \langle f_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{k}\downarrow} \rangle \langle f_{\mathbf{p}\downarrow} f_{\mathbf{p}\downarrow}^\dagger \rangle \right) \\ &\quad + \frac{\tilde{J}}{2V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) \left(\langle f_{\mathbf{k}\uparrow}^\dagger f_{\mathbf{k}\uparrow} \rangle \langle f_{\mathbf{p}\downarrow} f_{\mathbf{p}\downarrow}^\dagger \rangle + \langle f_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{k}\downarrow} \rangle \langle f_{\mathbf{p}\uparrow} f_{\mathbf{p}\uparrow}^\dagger \rangle \right) \\ &= \frac{3\tilde{J}}{2V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) n_{\mathbf{k}} (1 - n_{\mathbf{p}}) = -\frac{3\tilde{J}}{8V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) \cos 2\theta_{\mathbf{k}} \cos 2\theta_{\mathbf{p}}, \end{aligned} \quad (5.92)$$

where the last equality uses $\langle f_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma} \rangle = n_{\mathbf{k}}$, $\langle f_{\mathbf{p}\sigma} f_{\mathbf{p}\sigma}^\dagger \rangle = 1 - n_{\mathbf{p}}$, $2n_{\mathbf{k}} - 1 = \cos 2\theta_{\mathbf{k}}$, together with $\sum_{\mathbf{k}} \gamma(\mathbf{k} - \mathbf{p}) = 0$. The Hartree (direct) channel, obtained by contracting the two bilinears within each bracket, is instead proportional to the local magnetization and vanishes in the $SU(2)$ -symmetric state.

Anomalous contractions. Both the longitudinal and the transverse parts of (5.87) additionally admit contractions that pair the two creation operators with each other and the two annihilation operators with each other. With $\langle f_{\mathbf{k}\uparrow}^\dagger f_{-\mathbf{k}\downarrow}^\dagger \rangle = \Delta_{\mathbf{k}}$ and $\langle f_{-\mathbf{p}\downarrow} f_{\mathbf{p}\uparrow} \rangle = \Delta_{\mathbf{p}}$, we obtain

$$\begin{aligned} E_J^A &= -\frac{3\tilde{J}}{2V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) \langle f_{\mathbf{k}\uparrow}^\dagger f_{-\mathbf{k}\downarrow}^\dagger \rangle \langle f_{-\mathbf{p}\downarrow} f_{\mathbf{p}\uparrow} \rangle \\ &= -\frac{3\tilde{J}}{2V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) \Delta_{\mathbf{k}} \Delta_{\mathbf{p}} \\ &= -\frac{3\tilde{J}}{8V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{p}}, \end{aligned} \quad (5.93)$$

where, as for the normal channel, the four spin combinations produce the factor 3 and we used $\Delta_{\mathbf{k}} = \frac{1}{2} \sin 2\theta_{\mathbf{k}}$. Collecting the two channels,

$$E_J^{\text{SC}} = -\frac{3\tilde{J}}{8V} \sum_{\mathbf{k}\mathbf{p}} \gamma(\mathbf{k} - \mathbf{p}) (\cos 2\theta_{\mathbf{k}} \cos 2\theta_{\mathbf{p}} + \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{p}}), \quad (5.94)$$

to be minimized over $\{\theta_{\mathbf{k}}\}$ subject to the constraint (5.90).

The saddle point of (5.94) at finite doping is solved by a gap of d -wave symmetry, $\Delta_{\mathbf{k}} = \Delta_{\text{SC}} (\cos k_x - \cos k_y)$, recovering the d -wave BCS state quoted in the main text [Eq. (5.49) and following] [171, 188]. The same expression (5.94) governs the half-filled case relevant to the π -flux state of case B (5.50), obtained by setting $\delta = 0$ in the constraint (5.90).

Conclusions

At the core of this thesis lies the idea that, in strongly correlated systems, a quasiparticle description can remain a powerful organizing principle even when the conventional picture of electron-like excitations breaks down. The relevant effective quasiparticles need not be adiabatically connected to the bare electrons, nor must their spectrum coincide with the physical electron one. They may instead appear through zeros of the single-particle Green's function, or as auxiliary degrees of freedom within a variational representation of the many-body ground state. When appropriately constructed, such generalized quasiparticle descriptions provide a compact language in which topology, fractionalization, transport, and collective instabilities can be treated within a common framework.

Among the most intriguing possibilities proposed in this thesis is that the analytic structure of the single-particle Green's function may contain information beyond that carried by the conventional quasiparticles associated with its poles. In particular, zeros of the Green's function need not represent only a suppression of electronic spectral weight. They can signal emergent fractionalized excitations that are invisible in the single-particle spectrum, yet carry well-defined quantum numbers and nontrivial topology, as well as contribute to collective instabilities. Establishing the precise conditions under which this interpretation is valid remains an important open problem. A systematic characterization of the relation between Green's function zeros, fractionalized excitations, and their observable consequences would help clarify whether the phenomenology identified here extends broadly across Mott insulators [55, 57], topological Kondo insulators [61], and fractional Chern insulators [200].

This perspective extends naturally to the auxiliary one-body structures introduced in variational approaches such as the ghost-Gutzwiller method. The corresponding quasiparticle Hamiltonian provides a simple and intuitive description of both low- and high-energy physics in strongly correlated systems, retaining meaningful topological information even deep in the correlated regime. Our work suggests a route toward extending the concepts and tools of band topology beyond their conventional weakly interacting setting. The central challenge is therefore to establish which properties of the auxiliary description correspond directly to physical observables and which require additional many-body information.

In this context, topology provides a particularly stringent testing ground. Although an effective quasiparticle Hamiltonian may correctly encode the low-energy geometric properties of a correlated metal, nonquantized response functions are generally not determined by the quasiparticle spectrum alone. Residual interactions among quasi-

particles at the Fermi surface dress the current vertex and must therefore be properly taken into account. Developing a microscopic theory of these corrections constitutes a natural continuation of this work. Within Fermi-liquid theory, this requires controlled estimates of the Landau interaction parameters in realistic multiorbital systems, for example through a Hartree–Fock treatment combined with the random-phase approximation. A complementary route is provided by the ghost-Gutzwiller framework, which yields a variational description of both the correlated ground state and its low-energy excitations. In this setting, the central question is how the local variational operators dress physical observables, including the current, relative to their auxiliary quasiparticle counterparts. A consistent response theory of this kind would clarify both the predictive content and the limitations of generalized quasiparticle constructions.

Another promising direction is to exploit this auxiliary quasiparticle construction to investigate exotic phases in which topology and fractionalization coexist. The results presented in this thesis indicate that the ghost-Gutzwiller approach can describe fractionalized excitations, such as spinons, with vanishing physical-electron spectral weight. Combined with its ability to account for topological nontrivial features, this opens the route toward studying topological spin liquids in Mott insulators and the intriguing phases that emerge upon doping them. Such systems provide a natural setting in which to investigate how fractionalized excitations acquire electric charge, form Fermi surfaces, or condense into unconventional ordered states. Doped chiral spin liquids are especially compelling in this respect, as they may connect topological Mott physics to chiral superconductivity [201–203] through the dynamics and condensation of emergent quasiparticles.

Taken together, the results of this thesis support an expanded notion of quasiparticle, defined not by adiabatic continuity to the bare electron, but by its ability to encode robust structures within a correlated many-body state. Green’s function zeros and auxiliary quasiparticle Hamiltonians can reveal topology and fractionalized excitations that are not directly visible in the physical electron spectrum, while the analysis of response functions shows that their physical content is completed only after residual interactions and the dressing of observables are properly included. Further development of this framework may provide a unified approach to understanding how topology, fractionalization, and collective phenomena intertwine in strongly correlated electron systems.

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