

Development of a QMC code to tackle interacting electronic systems in 2D with application to TMD nanoribbons

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The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles.

P. W. Anderson

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Acknowledgments

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Abstract

The aim of this work (English)

Keywords

2D Materials, Hubbard Model, Strongly Correlated Electrons, Transition Metal Dichalcogenide Nanoribbons, Mean Field Theory, Determinant / Auxiliary Field Quantum Monte Carlo (QMC) (English)

Resumo

O objectivo deste trabalho (Português)

Palavras Chave

Materiais Bidimensionais, Modelo de Hubbard, Eletrões Fortemente Correlacionados, Nanofitas de Dicalcogenetos de Metais de Transição, Teoria de Campo Médio, Monte Carlo Quântico: Método do Determinante ou Campo Auxiliar (Português)

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Abbreviations

QMC Quantum Monte Carlo

TMD Transition Metal Dichalcogenide

LG Landau Ginzburg

2D Two-dimensional

1D One-dimensional

PBC Periodic boundary condition

OBC Open boundary condition

PHS Particle-hole symmetry

AF Antiferromagnetic

PHT Particle-hole transformation

AFM Atomic Force Microscopy

BSS Blankenbecler, Scalapino and Sugar

FFT Fast Fourier Transform

GCE Grand-canonical ensemble

TMDNR Transition Metal Dichalcogenide Nanoribbon

1

Introduction

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The isolation of graphene in 2004 has led to a growing interest of the scientific community in Two-dimensional (2D) materials revealing extraordinary properties. Among them, are Transition Metal Dichalcogenides (TMDs) appearing in the form of a variety of nanostructures. In these systems, electrons are strongly correlated, and one cannot neglect the interactions between them, unlike in graphene. Analytical approaches to the solution of the problem are either hopeless, or rely on possibly unrealistic approximations. In fact, the increased complexity of the models describing such highly correlated materials, compared to their graphene counterparts, calls for sophisticated computer simulation methods, most notably Quantum Monte Carlo (QMC). In this introductory chapter, we start by reviewing the literature on the physics of TMDs, focusing on their basic properties. Then, we present a survey of simulation methods belonging to the Quantum Monte Carlo class. We introduce some basic concepts, and motivate the choice of the particular used method. Finally, we summarize our original contributions, and outline the structure of the thesis.

1.1 Motivation

It might seem surprising that 2D systems were not considered as a real possibility before the discovery of graphene since they are often idealized in thought experiments, for example when investigating toy models of more complex higher dimensional systems. In fact, while thin film deposition on comparably thicker substrates was commonplace long before 2004, 2D layers were thought not to exist independently from their 3D base. Their existence was not expected *a priori* because at first sight they seem to violate the Mermin-Wagner-Hohenberg theorem [1–3], a no-go theorem that forbids ordering below three dimensions at finite temperature¹. The discovery of graphene paved the way for the search for similarly stable 2D materials, and since it was isolated, a plethora of these has been discovered. A vast set of open problems remains to be solved within the realm of the fascinating and counterintuitive properties of the now huge variety of existing 2D systems. In particular, in some of these, the effect of electron interactions is non negligible, leading to emergent phenomena. These are collective effects that emerge as a result of the interactions between the individual components of a system. The properties of the system’s components do not directly percolate up; instead, they shape the interactions that dictate the system’s properties sometimes in rather unexpected ways, leading to unusual behavior.

Interacting electron systems are often tackled by carrying out computer simulations. QMC is a family of numerical methods that are amply applicable to condensed matter physics problems, and that are particularly well suited to study strongly correlated electrons. Despite the system size being constrained due to limited simulation time, reliable, accurate and unbiased solutions are provided to the otherwise intractable quantum many-body problem. The class of QMC algorithms that is used in this work was introduced in the 1980’s in a series of seminal papers by Hirsch and Blankenbecler, Scalapino and Sugar² [4–10], but it saw a recent surge [11–23] due to the increase in computational power, and

¹2D materials can be stable because not all the conditions of Mermin-Wagner-Hohenberg theorem are verified, namely the condition of short-ranged interactions. In the particular case of graphene sheets, ripples appear, which implies that the material is not strictly 2D, and thus can be stabilized. The issue is subtle, and is beyond the scope of this work.

²After whom the Blankenbecler, Scalapino and Sugar (BSS) algorithm, on which we based the implementation used

algorithmic development. As a result, the field is currently very active. Method optimization can prove crucial in applications to widely studied physical models of electron interactions. In particular, recent computational and algorithmic developments opened the door to the study of both larger and lower temperature systems [14, 24–26].

In this work, an implementation of determinant QMC based on the BSS algorithm is used to simulate a TMD zigzag-edged nanoribbon, a nanostructure made of this recent member of the 2D materials family. Preliminary mean field studies show that this type of nanostructures have a tendency towards magnetism [27], which makes them good candidates for use in nanospintronics. QMC is a complementary, more accurate approach that can shed light upon these and other phenomena, like the formation of charge density waves and superconductivity.

1.2 Strongly correlated electron systems

Condensed matter physics is concerned with the emergence of the properties of quantum materials from complexity. The central concept within this approach is that of symmetry breaking. When a phase transition occurs, a system is said to condense into a phase of lower (or higher) symmetry. A simple pictorial example is the transition from a gas to a solid. Statistically, any point within a gas is equivalent, that is, on average, the surroundings of all points look similar. Formally, the system is then said to be fully translationally invariant. On the other hand, in a solid, a point is only equivalent to a discrete set of other points. In fact, a simplified view of a solid consists of a periodic arrangement of atoms occupying the points of a lattice. Any point on the lattice can be reached starting from any other point upon translation by a lattice vector. Thus, a system that makes a transition from the gaseous to the solid state becomes invariant only under a discrete set of translations, rather than a continuous one.

A framework that is commonly used to identify symmetry breaking is the Landau Ginzburg (LG) theory of phase transitions. The theory gives a prescription to discover phase transitions. More precisely, it gives criteria for a symmetry to become manifest. Although this framework is very useful, it turns out that the search for order relies on symmetry ideas well beyond condensed matter. Symmetry breaking gives rise to emergent phenomena. The idea of emergence rests on a constructionist, rather than a reductionist hypothesis: that the behavior of the many does not trivially follow from the behavior of the few. As P.W. Anderson puts it, “The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe.” [28]

The broad scope of condensed matter comes from the sheer number of possibilities that the symmetry breaking approach affords. For the specific case of the LG theory, one can study the emergence of magnetism, superconductivity, or superfluidity, just to name a few. However, as we shall see, sometimes the LG theory fails to capture a system’s behavior, and we must resort to other theories to identify these, or other eventual properties that might arise. The Landau Ginzburg procedure can be summarized as follows: identify an order parameter reflecting the underlying symmetry of the system, in this work, is named.

and minimize the free energy in order to deduce conditions for the symmetry to become manifest, leading to a phase transition. The drawback of this *variational* approach is that it might be difficult to identify an order parameter in the first place. Moreover, even if we do manage to find one, the usual procedure may be impossible to perform. It can easily happen that the degree of complexity of the order parameter is simply too high. Additionally, and perhaps more importantly, not all phase transitions can be described by the LG paradigm.

On the one hand, there are systems where a different kind of order arises. A prominent example is that of fractional quantum Hall effect, where (rather surprisingly!) the *quasi-particles* describing the excitations of the quantum Hall fluid carry *fractions* of the electron charge. There is an intimate connection between charge fractionalization and topology, which may be understood in terms of the properties of the Laughlin states describing the quantum Hall fluid. However, while it is tempting to try to characterize the latter in terms of the LG paradigm, it must actually be regarded as a distinct type of matter, where “topological order” arises [29].

On the other hand, for the so called strongly correlated systems we shall focus on in this work, there are phenomena which emerge specifically due to the interacting nature of the problem. They are elusive because a description in terms of the LG paradigm does not yield a behavior consistent with what is observed empirically. Instead, order emerges from the complexity created by the interactions among all the constituents. The LG theory fails because it ignores these interactions by disregarding fluctuations in the microscopic configuration of the system. This approximation consists of reducing the complex interactions to an effective *mean field*, which is normally determined self consistently. Strongly correlated systems require an approach beyond mean field, which makes them both extremely interesting and notoriously difficult to tackle. The mean field view fails to describe them because it considers each constituent to interact only with an external entity representing the interactions with all other constituents, underestimating collective behavior. In fact, the failure of mean field theory is not limited to correlated systems, and its success in describing a given system depends, for example, on the dimensionality³ and on the range of the particular type of interaction that is considered.

In many cases, mean field theory is too extreme an approximation. Nonetheless, its occasional failure at capturing the whole of a system’s properties does not deem it useless. Actually, it is quite the contrary. Mean field is often used as a first approach to build an intuitive physical picture for the general properties and behavior of the system. Of course, this is done while keeping in mind that the description it provides is intrinsically insufficient. Clearly, to extract the features of a correlated system we must extend it to the fully interacting case.

Strongly correlated quantum matter is ubiquitous and is at the heart of today’s most advanced electronic materials, namely organic conductors, high T_c (cuprate) superconductors, colossal magnetoresistance materials, and “heavy-fermion”⁴ compounds. Actually, the problem of strong correlations has now expanded beyond condensed matter physics. Quark-gluon plasmas, believed to have been formed just a few microseconds after the Big Bang, also belong to this class of systems. Another

³Normally, there is an upper critical dimension d_c above which mean field is exact. Below d_c , its predictions might be useful qualitatively, but not quantitatively.

⁴The quasi-particles describing excitations in these materials behave like much heavier electrons, hence the name.

example comes from atomic physics: ultracold atoms in optical lattices behave in a very similar way to correlated electrons. In fact, the behavior is so similar that these systems are being used as *de facto* quantum simulators of correlated electron systems [30].

A central piece in the understanding of correlated matter is the Hubbard model. It was introduced to bridge a gap between metals and magnetic insulators, building on the earlier work of Mott. The model is extremely simple. Electrons hop from atom to atom on a lattice, paying an energy penalty when they occupy the same site. This repulsive effect results in correlations beyond those that are always present due to the fermionic nature of the particles obeying the Pauli exclusion principle. In the limit of weak repulsion, the electrons are nearly free, and the system behaves like a metal. Otherwise, the electrons become localized at fixed atomic positions resulting in magnetic insulating behavior. The model is simple to formulate, but already includes highly nontrivial correlation effects between all electrons in the solid. Thus, it is not surprising that an exact solution exists only in 1D [31], and higher dimensional versions are still being studied more than 50 years after the model appeared [32].

1.3 Beyond graphene: TMD nanoribbons

2D materials have steadily been drawing the attention of the community since graphene was experimentally isolated from a graphite sample by mechanical exfoliation, yielding a system constituted by a single layer of atoms (Fig. (1.1), left). Since then, numerous studies have been made due to the promising properties of these materials, and the interesting as-yet-unseen phenomena occurring within them, for example, in the case of graphene: unconventional quantum Hall effect, absence of localization, and electrons behaving like massless relativistic particles near the K points, where the dispersion relation is approximately linear (Fig. (1.1), right), providing a bridge between condensed matter physics and quantum electrodynamics [33]. In spite of its undeniable potential, graphene has some shortcomings. This motivated the community to study other more complex graphene-like materials, which could have other desirable properties, while maintaining most of graphene's potential.

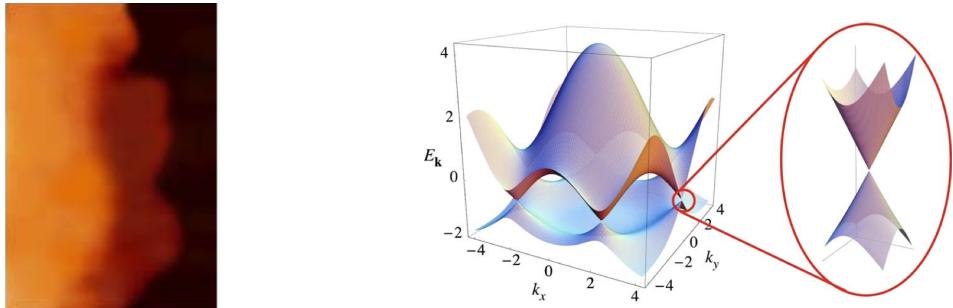


Figure 1.1: Left: Atomic Force Microscopy (AFM) picture of a graphene monolayer. The black area is a substrate used for fabrication purposes. The dark orange area is a monolayer of graphene. Right: Dispersion relation of graphene. The Fermi energy is set to zero. Close to it, the dispersion relation is linear, corresponding to massless excitations (taken from [34]).

TMDs are prominent examples of such novel members of the 2D materials family [35–37]. An excellent review of their properties, experimental results and applications is given in [38]. Much like graphite which is essentially constituted by stacked monolayers of carbon atoms bound by weak Van der

Waals forces, 3D TMD structures are also formed by weakly bound layers. However, instead of carbon, the layers contain transition metals M , and chalcogens X , in a two X to one M proportion. Thus, group 6 TMDs are denoted MX_2 , where $M = \text{Mo}, \text{W}, \dots$ (respectively Molybdenum and Tungsten) and $X = \text{S}, \text{Se}, \text{Te}$ (respectively Sulfur, Selenium and Tellurium). Each monolayer contains a layer of M atoms organized in a triangular lattice sandwiched between two layers of X atoms, as opposed to graphene, where carbon atoms are all on the same plane. Each M atom is coordinated with six X atoms, giving rise to a stacked structure with various possible coordinations, depending on the spatial arrangement of the X atoms. The most common structural phases are trigonal prismatic (2H) and octahedral (1T). TMD monolayers are still considered 2D since their thickness is at the atomic scale. For example, for molybdenum disulfide, MoS_2 , monolayers are only 6.5\AA thick. For this reason, for the particular case of the 2H phase we shall focus on from now on, the $M - X$ lattice is thought of as being hexagonal, as seen in the top-down view of Fig (1.2a). Valence bands arise out of the hybridization of the d_{xy} and $d_{x^2-y^2}$ orbitals of the transition metal and the $p_{x,y}$ orbitals of the chalcogen, while conduction bands have a main contribution from the $d_{3z^2-r^2}$ orbitals of the M atoms with only a minor contribution from the $p_{x,y}$ orbitals of the X atoms.

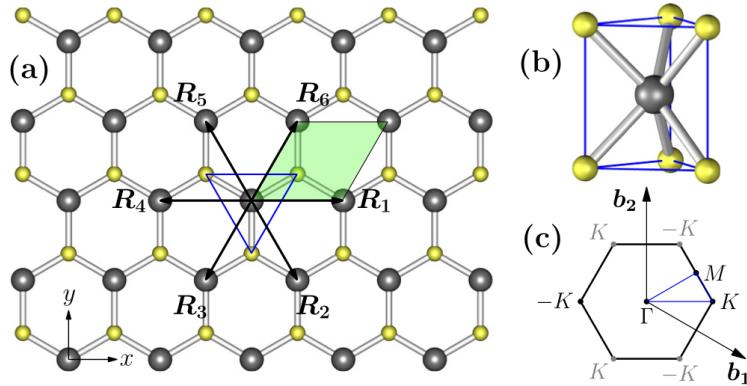


Figure 1.2: (a) The 2H phase of a TMD monolayer may be viewed simply as a $M - X$ honeycomb lattice. Here we represent the six nearest neighbors of a point on the M triangular lattice by the real space vectors $\mathbf{R}_{i=1,2,\dots,6}$. (b) Unit cell of the trigonal prismatic (2H) phase of a TMD monolayer. (c) High symmetry points Γ, M, K of the first Brillouin zone ($\mathbf{b}_{1,2}$ are the reciprocal basis vectors).

2D TMDs have been attracting interest because they seem to overcome some of the drawbacks of graphene in technological applications. For example, monolayer graphene is gapless, while its bilayer counterpart has a tunable, but small gap of the order of a tenth of an eV. Contrastingly, monolayer TMDs are semiconductors, having an intrinsic gap in excess of 1 eV, which lies at the inequivalent K points of the hexagonal Brillouin zone. Thus, TMDs are more promising for designing, for example, transistors. More generally, since the direct band gap lies in the visible frequency range, and room temperature mobility is good, these semiconducting analogues of graphene are promising for electronic and optoelectronic applications. Perhaps even more striking is the appearance of an extra so called *valley* degree of freedom. Since the valence and conduction band edges both lie at the two corners ($\pm K$) of the first Brillouin zone, electrons and holes can acquire a novel degree of freedom which can be used to encode and process information. Additionally, the presence of giant spin-orbit coupling and the lack of inversion symmetry lead to a strong coupling between valley and spin, suggesting that

TMDs could allow the integration of spintronics and valleytronics.

Hole-doped TMDs are expected to show topological superconductivity [39], while the superconducting phase of graphene has been predicted, but is not easily attained. Superconductivity in graphene-like 2D materials is important because it could boost high speed nanoelectronics. Moreover, the presence of transition metal atoms in TMDs suggests the possibility of magnetic ordering [40], which could be very relevant in nanospintronics applications. Both superconductivity and magnetic ordering may arise due to the effect of strong electron correlations. Thus, to investigate these properties of TMDs reliably, we need a computational method that is robust enough to capture the effects of strong electron interactions accurately. As we shall see, auxiliary field QMC fulfills this criterion.

1.3.1 Electronic properties

The electronic properties of TMD monolayers depend crucially on the coordination. In particular, for the 2H phase, they may ultimately be attributed to the lack of inversion symmetry relative to the M atoms. This leads to spin splitting of the electronic bands driven by spin-orbit coupling. Because K and K' (or $-K$) no longer correspond to time reversal invariant momenta, the spin degeneracy of the valence and conduction bands is lifted at these points. Time reversal symmetry implies that the splitting is opposite at the K and K' points, leading to the band structure of Fig. (1.3d) (we show the part relevant for realistic charge-carrier concentrations).

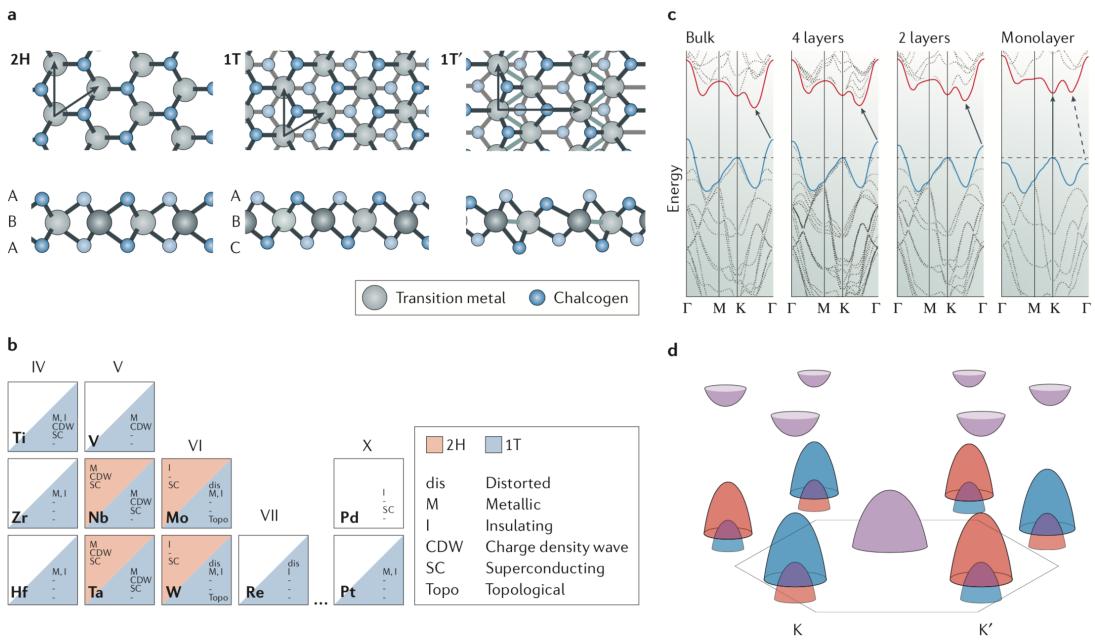


Figure 1.3: (a) Examples of some of the possible structural phases of TMD monolayers: trigonal prismatic (2H) with ABA stacking, distorted octahedral (1T), and dimerized octahedral (1T'), showing ABC stacking. (b) A periodic table of known TMD layers. Shown are the transition metals involved, the existing phases (2H and/or 1T), and the possible electronic phases. (c) Calculated band structure (from density functional theory [41]) of 2H – MoS₂ for samples of decreasing thickness. (d) Representation of the band structure of monolayer 2H – MoS₂, showing the spin splitting (red for spin-up and blue for spin-down) of the bands near the corners of the Brillouin zone (K and K') points.

This property, known as spin-valley coupling, implies that the valley polarization of charge carriers directly translates into spin polarization, leading to an intrinsic property of TMDs that could allow one

to design spintronic devices without resorting to magnetic materials [38]. More broadly, the possibilities afforded by the different compositions and structural phases listed in Fig.(1.3) lead to a vast array of electronic properties. On the one hand, the band structure and its metallic/insulating character vary quite substantially among TMDs. On the other hand, both highly nontrivial correlated and topological phases arise within these materials. In this work, we investigate the properties of correlated phases in zigzag edged TMD nanoribbons.

1.3.2 Nanoribbons

Nanoribbons are a particularly promising type of 2D nanostructure. A nanoribbon consists of a 2D layer that can be regarded as infinitely long on one direction, but not on the other (Figs. (1.4) and (1.5)), so that edge states become relevant, and can be controlled to yield interesting properties. For simulation purposes, it is natural to assume translational invariance along the ribbon's longitudinal direction, and use Periodic boundary conditions (PBCs). On the other direction, we use Open boundary conditions (OBCs), effectively considering zigzag edges (see Fig.(1.6), left).

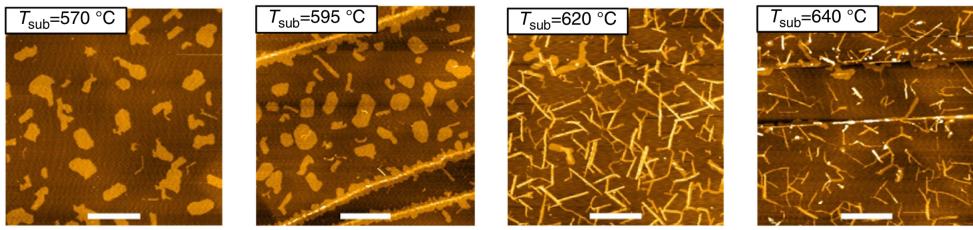


Figure 1.4: Fabrication of TMD nanoribbons. From left to right, we see AFM images showing the appearance of nanostructures ranging from 2D nanoislands to nanoribbons, as the temperature of the substrate is increased. The nanoribbons are grown by taking advantage of the temperature dependence of shape transformations occurring during the nonequilibrium growth of surface-based nanostructures (taken from [42]).

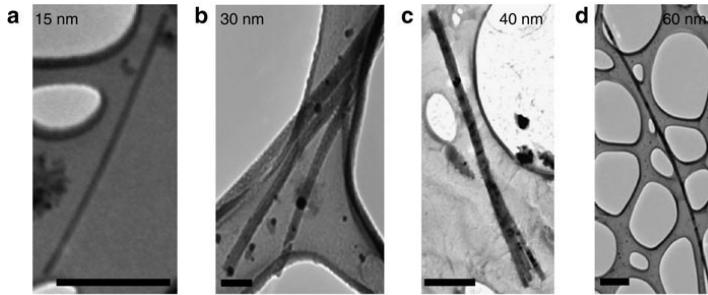


Figure 1.5: (a) to (d) - Transmission electron microscopy (TEM) images of graphene nanoribbons (GNRs) of widths 15, 30, 40, and 60 nm, respectively (adapted from [43]).

A high density of low-energy electronic states is localized at the zigzag edges, decaying quickly in the bulk, which suggests the possibility of magnetic ordering. In fact, a mean field solution of the Hubbard model for a graphene nanoribbon shows that magnetic moments are localized at the edges [27] (see Fig.(1.6), right). QMC has been used to investigate edge-state magnetism beyond mean field in graphene [44–48]. However, edge-state magnetism in TMDs remains unexplored [49], and we would like to investigate, for example, whether edge-state magnetism is stabilized at finite temperature in Transition Metal Dichalcogenide Nanoribbons (TMDNRs), following the tendency that was identified

for their graphene counterparts.

While the zigzag graphene nanoribbon antiferromagnetic ground state is semiconducting, a state with interedge ferromagnetic orientation is a metal. An example of an application based on the switching between the two states is a magnetoresistive sensor. This device allows switching between low and high-resistance configurations, corresponding, respectively, to parallel, and antiparallel configurations of ferromagnetic leads at the ends of a nanoribbon. An analogous form of edge-state magnetism, as is observed in graphene nanoribbons, for TMDNRs, could yield similarly innovative applications.

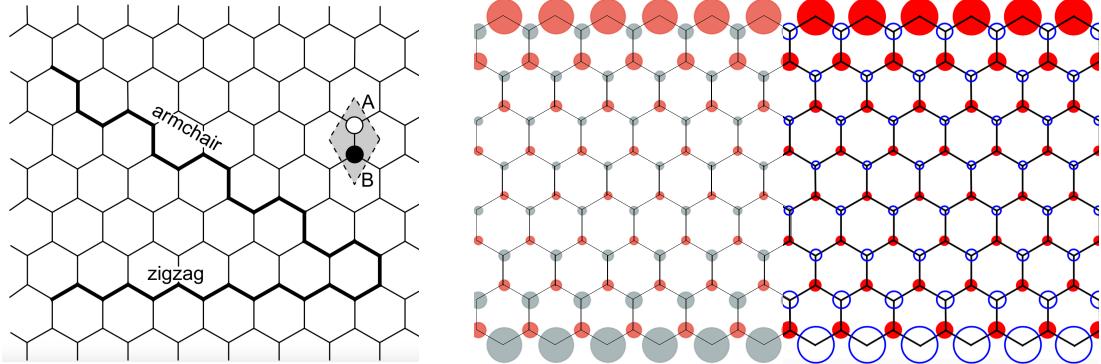


Figure 1.6: Left: Two possible terminations of a TMD nanoribbon condensing in a honeycomb lattice. Right: Example of a mean field result for a graphene nanoribbon. Local magnetic moments tend to develop significantly on zig zag edges. The area of the circles corresponds to the magnitude of the magnetic moment. The red circles corresponds to the spin up density, and the blue ones to the spin down density. The particular arrangement of the electronic edge states leads to an AF ground state (opposite edges with opposite magnetic moment). The results on the right part of the picture are taken from [27], while the left part corresponds to our original results clearly reproducing the ones on the literature).

1.3.3 Effective three-band minimal tight-binding model

In this section, we present a minimal model describing the low energy physics of group 6 TMD monolayers [50]. To obtain this tight-binding model, one uses the symmetries of the monolayers, and the fact that conduction and valence band edges have major contributions from d_{z^2} , d_{xy} , and $d_{x^2-y^2}$ orbitals of M-atoms at the K points. This is illustrated for MoS₂ in Fig.(1.7). Near the Fermi energy, the Mo d -orbitals are clearly more populated at the K point (circled in orange), hence these Bloch states contribute more to the energy dispersion near that point.

One of the members of the D_{3h} point-group describing the symmetry of TMD monolayers is the reflection operator by the $x - y$ plane (see Fig.(1.2)). This imposes the restriction that hybridization occurs only between the d_{z^2} , d_{xy} , and $d_{x^2-y^2}$ orbitals⁵, which motivates us to construct a three-band model. Moreover, the dimension of the irreducible representation of D_{3h} imposes a constraint on the number of independent hopping parameters. By fitting to first principles results obtained from density functional theory (using both the local-density and the generalized gradient approximations - LDA and GCA) for the materials' energy bands, we obtain the hopping parameters. The strategy that is chosen to do the fit in [50] is to fit the band energies at the high-symmetry k -points Γ , K , and M , and

⁵ d_{yz} and d_{xz} orbitals are not symmetric under reflection upon the $x - y$ plane.

the energies of the valence and conduction bands near K by least-squares. This procedure leads to a non-uniform nearest neighbor (NN) hopping matrix on the M-atom triangular lattice.

Note that since the argument is purely based on symmetry, in general, the $d - d$ hoppings include both direct $d - d$ interactions of M atoms, and indirect ones, mediated by $X - p$ orbitals. These M-M hoppings suffice to describe the band-edge properties near the $\pm K$ valleys. By including third nearest neighbor hoppings, one can reproduce the energy dispersion in the entire first Brillouin zone.

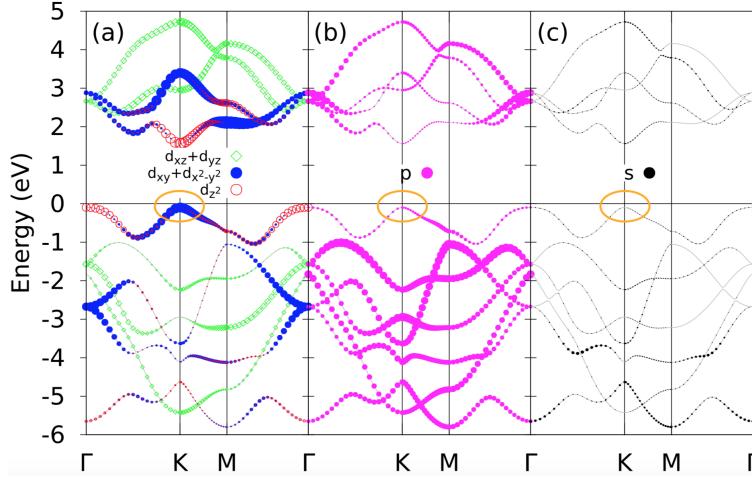


Figure 1.7: Orbital projected band structures for monolayer MoS₂ obtained from first principles. The Fermi energy is set to 0, and the symbol size is proportional to the population of the state. The panels represent the contributions from: (a) Mo d -orbitals; (b) All p -orbitals, dominated by S atoms; (c) All s -orbitals.

We start by introducing the “spinless” model, and then generalize it to include spin-orbit coupling. Let the greek indices represent orbital space, except for σ , meaning spin. Then, the Hamiltonian reads

$$\mathcal{H} = \sum_{i,j,\sigma} \sum_{\alpha,\beta} c_{i,\alpha}^\dagger t_{\alpha\beta}^\sigma (\mathbf{R}_i - \mathbf{R}_j) c_{j,\beta} = \sum_{i,j} \sum_{\alpha,\beta} c_{i,\alpha}^\dagger t_{\alpha\beta} (\mathbf{R}_i - \mathbf{R}_j) c_{j,\beta}, \text{ since } t_{\alpha\beta}^\sigma (\mathbf{R}) = t_{\alpha\beta}^\downarrow (\mathbf{R}) \equiv \frac{1}{2} t_{\alpha\beta} (\mathbf{R}) \quad (1.1)$$

where we consider the basis set $\{|\alpha\rangle\}_{\alpha=1}^3 = \{(d_{z^2}), (d_{xy}, d_{x^2-y^2})\}$. Here, we split the basis into two orbital categories based on which irreducible representation of the D_{3h} group they belong to. Let index j run through the orbital categories, and μ through the basis elements, so that the orbitals $|\phi_\mu^j\rangle$ are

$$|\phi_1^1\rangle = d_{z^2} \quad |\phi_1^2\rangle = d_{xy} \quad |\phi_2^2\rangle = d_{x^2-y^2} \quad (1.2)$$

By symmetry, there are eight independent parameters, which we choose as some of the hopping integrals $t_{\mu\nu}^{jk}(\mathbf{R}_i) = \langle \phi_\mu^j(\mathbf{r}) | \mathcal{H} | \phi_\nu^k(\mathbf{r} - \mathbf{R}_i) \rangle$. The remaining ones can be obtained from $t^{jk}(\mathbf{G}_n \mathbf{R}_i) = \mathbf{D}^j(\mathbf{G}_n) t^{jk}(\mathbf{R}_i) [\mathbf{D}^k(\mathbf{G}_n)]^\dagger$, where $\mathbf{D}_j(\mathbf{G}_n)$ is the $N_j \times N_j$ matrix of the j -th irreducible representation, and the \mathbf{G} -matrices are a subset of the symmetry operations of the D_{3h} group [50, 51]. Let

$$\begin{aligned} \varepsilon_1 &= t_{11}^{11}(\mathbf{0}) & \varepsilon_2 &= t_{22}^{11}(\mathbf{0}) = t_{22}^{22}(\mathbf{0}) & t_0 &= t_{11}^{11}(\mathbf{R}_1) & t_1 &= t_{11}^{12}(\mathbf{R}_1) \\ t_2 &= t_{12}^{12}(\mathbf{R}_1) & t_{11} &= t_{11}^{22}(\mathbf{R}_1) & t_{12} &= t_{12}^{22}(\mathbf{R}_1) & t_{22} &= t_{22}^{22}(\mathbf{R}_1) \end{aligned} \quad (1.3)$$

The on-site energies ε_j corresponding to the atomic orbitals $|\phi_\mu^j\rangle$ appear through a diagonal hopping matrix in orbital space $\mathbf{t}(\mathbf{0}) = \text{diag}(\varepsilon_1, \varepsilon_2, \varepsilon_2)$, while the NN hoppings are (see Fig.(1.2))

$$\mathbf{t}(\mathbf{R}_{1,4}) = \begin{pmatrix} t_0 & \pm t_1 & t_2 \\ \mp t_1 & t_{11} & \pm t_{12} \\ t_2 & \mp t_{12} & t_{22} \end{pmatrix} \quad (1.4)$$

$$\mathbf{t}(\mathbf{R}_{2,5})_{(3,6)} = \begin{pmatrix} t_0 & \pm \left(\pm \frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2 \right) & \mp \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 \\ \mp \left(\mp \frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2 \right) & \frac{1}{4}(t_{11} + 3t_{22}) & \pm \left(\frac{\sqrt{3}}{4}(t_{22} - t_{11}) \mp t_{12} \right) \\ \pm \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2 & \pm \left(\frac{\sqrt{3}}{4}(t_{22} - t_{11}) \pm t_{12} \right) & \frac{1}{4}(3t_{11} + t_{22}) \end{pmatrix} \quad (1.5)$$

The heavy transition metal M-atoms have large spin-orbit coupling, which persists in MX_2 monolayers. We model it by a minimal on-site term $\lambda \mathbf{L} \cdot \mathbf{S}$ for M-atoms that does not mix up and down-spins. Thus, the “on-site matrices” become spin-dependent, while the $t_{\alpha\beta}^\sigma(\mathbf{R}_i \neq \mathbf{0})$ remain unchanged. This is shown by acting with $\lambda \mathbf{L} \cdot \mathbf{S}$ upon our basis states explicitly. Although this produces states outside of the Hilbert space, these can be safely projected out since they are not allowed by symmetry [50, 51].

$$t_{\alpha\beta}^\sigma(\mathbf{0}) \rightarrow t_{\alpha\beta}^\sigma(\mathbf{0}) + \frac{\sigma\lambda}{2} \mathbf{L}_0, \quad \mathbf{L}_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 2i \\ 0 & -2i & 0 \end{pmatrix}, \quad \text{where } \sigma = \pm 1 \quad (1.6)$$

Spin-orbit coupling is important because it is responsible for the splitting of the valence band maximum by $\Delta_{\text{SOC}}^v = 2\lambda$. The conduction band minimum remains degenerate (although a finite small splitting Δ_{SOC}^c arises when considering perturbations due to the d orbitals that are not considered in our minimal model).

The minimal model we presented is very rich, and can be used to study many-body physics, for example by adding Hubbard-type interaction terms. Moreover, it can be used to study edge state physics by imposing appropriate boundary conditions on the hopping matrix. We will follow this route by numerically solving an interacting extension of the model for a nanoribbon using QMC.

1.4 Introduction to Quantum Monte Carlo

Solving the many-body problem remains one of the greatest challenges in physics. Following the wealth of attempts at such pursuit, certain phenomena arising due to the strong interactions in quantum systems are explained in different theoretical frameworks, namely superconductivity, the Mott metal-insulator transition, and fractional quantum Hall effect. All of these breakthroughs represented revolutions in their respective fields with significant scientific and technological impact.

Only in very limited cases does an actual analytical solution exist for the Schrödinger equation for a system of interacting particles. One must resort to sophisticated approximation methods to obtain information about the role played by the competing interactions under various conditions in the aforementioned cases. It is then natural that numerical methods have become prominent as a tool

for extracting useful information about this type of systems. QMC is amongst the most accurate and extensively studied ones. The idea of all QMC methods is to reduce the interacting problem to solving a set of integrals, which can be evaluated numerically through a standard stochastic procedure. These integrals are arrived at upon formulating the quantum many-body description of the system using the Schrödinger equation. Hence the name Quantum Monte Carlo, which is used to distinguish it from Classical Monte Carlo. In the classical version, one measures thermal averages, while in the quantum version, one measures expectations of operators over the Hilbert space of the system, corresponding to physical observables that fluctuate with a dynamics given by the Schrödinger equation.

The dynamics of a quantum system are encoded in the Hamiltonian operator. In the case of graphene-like 2D materials, one usually uses a tight-binding type of model. It is found that the dynamics given by the tight-binding Hamiltonian is sufficient to describe most properties of graphene. However, in other materials, such as TMDs, electron-electron interactions are stronger, and we must consider Hubbard-type models.

In principle, the properties of a quantum many-fermion system can all be deduced by solving an extremely complicated Schrödinger equation that takes into account the coupling of all (identical) particles of the system. However, for the majority of systems the resulting integrals have no analytic solution, so we solve the problem by numerical integration. But there is a myriad of methods to evaluate integrals numerically. How do we pick the best one for this case? Multi-dimensional integrals are plagued by the curse of dimensionality. Although the Newton-Cotes quadrature formulas (including, for example the Newton method, and Simpson's rules), Gaussian quadrature formulas, or Romberg's method all scale polynomially with the number of integration points, they become impractical as the dimension increases. To use them, one would invoke Fubini's theorem to reduce the multi-dimensional integral to a series of one-dimensional integrals. However, the number of function evaluations required to compute the whole integral grows exponentially with its dimension. The Monte Carlo method preserves the polynomial scaling, thus yielding comparable accuracy with far less function evaluations. It is natural to use it since typically the state space of our quantum system is huge, leading to high dimensional integrals.

The Monte Carlo method is ubiquitous. Its central idea is to use randomness to produce accurate estimates of deterministic integrals. The term was coined by Nicolas Metropolis in 1949, first appearing in a seminal paper, in which it was described as a “statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of sciences”[52]. Although it was used as early as 1777 in an experiment known as Buffon’s needle - where one obtains an estimate of the constant π by repeatedly throwing a needle randomly onto a sheet of paper with evenly spaced lines - it was crucially developed in the Los Alamos National Laboratory during World War II where the development of the first atomic bomb was completed, the primary objective of the Manhattan Project. The method is particularly useful when one wants to sample from a probability distribution in an exponentially large state space, but it can, in principle, be used to solve any problem allowing a probabilistic formulation.

A variety of QMC methods exists, using a sampling scheme based on the Metropolis algorithm,

and variations thereof. Variational and Diffusion QMC are the simplest QMC methods that allow one to capture the properties of correlated systems. Although they already contain the main concepts used in this type of simulations, it is not always ideal or even possible to use them. We will discuss their flaws and show how further refinement leads to the auxiliary field method we ultimately used.

Using the Monte Carlo approach to study a many-fermion system implies overcoming a significant obstacle common to all QMC methods - the so called *fermion sign problem*. Pauli's exclusion principle implies that the many-fermion wave function is anti-symmetric, which leads to a sign oscillation that greatly impedes the accurate evaluation of averages of quantum observables. The anti-symmetry constraint implies that a straightforward weight interpretation of the wave function is not possible. In the case of the finite temperature algorithm, the cancellations that occur when computing the average of any physical observable lead to poor statistical properties of the corresponding estimators. This means that a massive amount of samples requiring enormous computer time are needed to obtain meaningful results. In the case of the zero temperature algorithms, the situation is even worse. It might not even be possible to design a stochastic process carrying the system to its ground state, as normally is done in "projective" methods⁶: the wave function that is used as an initial proposal turns out to converge to a bosonic one, and the fermionic character of the system is lost.

As was proven by Troyer, the *fermion sign problem* has NP⁷ computational complexity [53]. One of the greatest open questions in computer science is whether $P = NP$. Solving the *fermion sign problem* would imply finding a solution to $P = NP$, which would constitute a major breakthrough.

1.4.1 Variational Monte Carlo

Variational techniques rely on an educated guess for the wave function of the system. One introduces a set of variational parameters α that are then tuned according to a variational principle. Then, we may use the optimized trial wave function to compute physical quantities of interest using Monte Carlo. The method is used to obtain zero temperature properties of a given model. Note that it requires prior knowledge about the system to propose an approximate wave function in the first place.

A particularly relevant observable is the variational energy E_V associated to a trial ground state. Let \mathbf{r} be the $3N$ spatial coordinates of the N electrons. For simplicity, let us ignore all other degrees of freedom, such as spin. Given the Hamiltonian of the system \mathcal{H} , and a trial wave function $\psi_T(\mathbf{r})$ - a guess of the wave function representing the ground state - one can compute the corresponding variational energy.

$$E_V = \frac{\langle \psi_T | \mathcal{H} | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} = \frac{\int d\mathbf{r} |\psi_T(\mathbf{r})|^2 E_L(\mathbf{r})}{\int d\mathbf{r} |\psi_T(\mathbf{r})|^2} = \int d\mathbf{r} \rho(\mathbf{r}) E_L(\mathbf{r}), \quad (1.7)$$

where

$$E_L = \frac{\mathcal{H}\psi_T(\mathbf{r})}{\psi_T(\mathbf{r})} \quad \text{and} \quad \rho(\mathbf{r}) = \frac{|\psi_T(\mathbf{r})|^2}{\int d\mathbf{r}' |\psi_T(\mathbf{r}')|^2} \quad (1.8)$$

⁶Methods that iteratively project a trial wave function onto the ground state.

⁷NP or nondeterministic polynomial time, meaning that one can devise an algorithm that verifies the "yes" answer to a decision problem in polynomial time in the system size. Note that the class P - of polynomial time algorithms - is a subclass of NP.

Note that we managed to recast the variational energy as an average of the *local* energy, $\langle E_L \rangle$, over the distribution ρ . This may be computed using the Monte Carlo method by sampling M points \mathbf{r}_k from the distribution $\rho(\mathbf{r})$. Denoting the sample mean of the random variable X as \bar{X} :

$$E_V \approx \bar{E}_L = \frac{1}{M} \sum_{k=1}^M E_L(\mathbf{r}_k), \quad (1.9)$$

Let the ground state energy be E_0 . Then, states are optimized according to the variational principle:

$$E_V(\boldsymbol{\alpha}) = \frac{\langle \psi_{\boldsymbol{\alpha}} | \mathcal{H} | \psi_{\boldsymbol{\alpha}} \rangle}{\langle \psi_{\boldsymbol{\alpha}} | \psi_{\boldsymbol{\alpha}} \rangle} \geq E_0, \quad (1.10)$$

where $\psi_{\boldsymbol{\alpha}}$ is the trial ground state wave function for the set of variational parameters $\boldsymbol{\alpha}$.

By varying $\boldsymbol{\alpha}$ we aim to obtain a variational energy that is as close as possible to the true ground state energy. Since $E_V(\boldsymbol{\alpha})$ is bounded from below, this is equivalent to minimizing it in the hope that $E_V(\boldsymbol{\alpha}_{min}) \gtrsim E_0$, i.e. the bound is tight. The finite sampling size M , of course, introduces a statistical error common to all Monte Carlo methods. However, the use of an approximate wave function introduces a systematic error that is hard to control since trial wave functions are generally introduced based on approximate, or heuristic arguments.

1.4.2 Diffusion Monte Carlo and projective methods

Variational Monte Carlo is severely limited by the use of a trial wave function $\psi_T(\mathbf{r})$ because we may not even have enough information to even construct a reliable variational wave function in the first place. Diffusion QMC allows the simulation of a many-body system while having only a limited knowledge of the system's physical properties. While it is exact for many-boson systems, it is only approximate for many-fermion systems. The idea is to map the Schrödinger equation onto an imaginary-time diffusion equation. Excited states are then filtered out by a diffusion process as we advance in imaginary-time. In imaginary-time $\tau = it$, the solution to the Schrödinger equation in terms of a formal series expansion in the eigenfunctions of the Hamiltonian becomes a series of “transient” wavefunctions weighted by $e^{-E_n \tau}$, $n \in \mathbb{N}$. Within precision and accuracy constraints, the longest lasting of these is the ground state [54]. Thus, the idea of the diffusion method is to generate samples using the exact ground state wave function $\psi_0(\mathbf{r})$ [55]. The associated exact energy E_0 is the matrix element of the hamiltonian calculated using a trial wave function and the ground state.

$$E_0 = \frac{\langle \psi_0 | E_0 \mathbb{1} | \psi_T \rangle}{\langle \psi_0 | \psi_T \rangle} = \frac{\langle \psi_0 | \mathcal{H} | \psi_T \rangle}{\langle \psi_0 | \psi_T \rangle} = \frac{\int d\mathbf{r} \psi_0^*(\mathbf{r}) \psi_T(\mathbf{r}) E_L(\mathbf{r})}{\int d\mathbf{r} \psi_0^*(\mathbf{r}) \psi_T(\mathbf{r})} \quad (1.11)$$

Note that using this trick we avoid the computation of $\mathcal{H}\psi_0 = E_0\psi_0$, that is, the ground state energy. Instead, we approximate the integral by considering M configuration samples $\mathbf{r}_{k=1,\dots,M}$ in a similar spirit to that of Variational QMC. Notice that the integral consists of a local energy of the trial wave function $E_L(\mathbf{r}) = \frac{\mathcal{H}\psi(\mathbf{r})}{\psi(\mathbf{r})}$ averaged over a mixed distribution from which we draw a sample:

$$f(\mathbf{r}) = \frac{\psi_0^*(\mathbf{r}) \psi_T(\mathbf{r})}{\int d\mathbf{r} \psi_0(\mathbf{r}) \psi_T(\mathbf{r})} \quad (1.12)$$

Although the method is, of course, aimed at probing many-body systems, let us consider a single particle in 1D, for simplicity, to illustrate the method. Performing a Wick rotation - effectively going to imaginary time - and shifting the energy, the Schrödinger equation becomes (with $\hbar = 1$)

$$\frac{\partial \psi_T(x, \tau)}{\partial \tau} = -\frac{1}{2m} \frac{\partial^2 \psi_T(x, \tau)}{\partial x^2} - \left[V(x) - E_T \right] \psi_T(x, \tau) \quad (1.13)$$

The exact ground state wave function $\psi_0(x)$ is obtained as the longest lasting transient state in imaginary time: we are interested in the asymptotic behavior of the series expansion constituting the formal solution of the Schrödinger equation

$$\psi_T(x, \tau) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-(E_n - E_T)\tau} \quad (1.14)$$

Imaginary time evolution is governed by

$$|\psi_T(t)\rangle = \lim_{\tau \rightarrow \infty} \sum_n e^{-(E_n - E_T)\tau} |\psi_n\rangle \langle \psi_n| \psi_T \rangle = \lim_{\tau \rightarrow \infty} e^{-(E_0 - E_T)\tau} |\psi_0\rangle \langle \psi_0| \psi_T \rangle \quad (1.15)$$

If $E_T > E_0$ the wave function diverges exponentially fast: $\lim_{\tau \rightarrow \infty} \psi_T(x, \tau) = \infty$. Similarly, for $E_T < E_0$ it vanishes exponentially fast: $\lim_{\tau \rightarrow \infty} \psi_T(x, \tau) = 0$. However, if $E_T = E_0$ the wave function converges to the ground state one up to a constant factor, $c_0 = \langle \psi_0 | \psi_T \rangle$.

$$\lim_{\tau \rightarrow \infty} \psi_T(x, \tau) = c_0 \psi_0(x) \quad \text{or} \quad \lim_{\tau \rightarrow \infty} |\psi_T(\tau)\rangle \propto |\psi_0\rangle \quad (1.16)$$

Diffusion QMC makes use of Eq. (1.16), approximating $\psi_0(x)$ by $\psi_T(x, \tau)$ for sufficiently long time. The only requirement is that $\psi_T(x, \tau)$ and $\psi_0(x)$ overlap significantly so that c_0 is large enough to be numerically measurable, and we can always center a positive trial wave function in a region where $\psi_0(x)$ is large enough and positive. If the latter condition does not hold, the wave function converges to a bosonic, instead of a fermionic one. Of course, these conditions can always be met for a single particle, but note that they might fail for a many-fermion system, for which the wave function crosses a number of nodes due to its anti-symmetric nature.

1.4.3 Auxiliary Field QMC and the Fermion Sign Problem

As we have seen, the major drawback of the variational method was that it demanded *a priori* knowledge of a reasonable variational wave function describing, at least partly, some of the physics of the problem. Diffusion QMC demands less: we need only propose a trial wave function that overlaps with the ground state. However, none of these methods allow us to probe systems at finite temperature. Moreover, they both require some prior knowledge about the system, which may not always be available.

An alternative method is based on introducing an additional lattice bosonic field that mediates the electron-electron interaction. The interacting problem then becomes a problem of independent fermions coupled to an external field, and the fermionic part of the partition function can be traced out

explicitly, leaving the contribution of a *discrete*⁸ bosonic field, \mathbf{h} . This contribution can be evaluated numerically by employing importance sampling over the field configurations. Auxiliary field QMC relies on a mapping to a “classical” system (in quotes because there is no actual classical analogue):

$$Z = \text{Tr}[e^{-\beta \mathcal{H}}] = \sum_{\{\mathbf{h}\}} \sum_{\text{fermionic}} e^{-S} = \sum_c p_c, \quad (1.17)$$

but some of the “probabilities” can actually be negative $p_c < 0$. This occurs due to the antisymmetry of the many-electron wavefunction under electron exchange, and is at the root of the sign problem. Here, S is a fermion-boson action that we shall write out explicitly later. For a fixed configuration of the bosonic field, we sum over the fermionic part exactly to obtain the weight of each configuration p_c . The sum over \mathbf{h} is carried out stochastically.

The negative weight problem may easily be circumvented when computing averages of observables:

$$\langle A \rangle = \frac{\sum_c A(c)p(c)}{\sum_c p(c)} = \frac{\sum_c A(c)|p(c)|\text{sign}[p(c)]/\sum_c |p(c)|}{\sum_c |p(c)|\text{sign}[p(c)]/\sum_c |p(c)|} \equiv \frac{\langle As \rangle_{|p|}}{\langle s \rangle_{|p|}}, \quad (1.18)$$

where $s(c) = \text{sign}[p(c)]$, and $|p(c)|$ corresponds to an auxiliary bosonic system (also coupled to the bosonic field) corresponding to the original fermionic system, and for which there is no sign problem.

The relative error $\Delta s / \langle s \rangle$ increases exponentially with the number of particles, with inverse temperature, and possibly with other parameters of the specific model to be studied [53, 56]. To see this, we start by noting that the average sign is the ratio between the partition functions of the fermionic ($Z = \sum_c p(c)$) and bosonic systems ($Z' = \sum_c |p(c)|$). In terms of the difference in free energy densities, $\langle s \rangle = Z/Z' = e^{-\beta N_p \Delta f}$, implying that for M samples, the error of the denominator of Eq. (1.18) becomes

$$\frac{\Delta s}{\langle s \rangle} = \frac{\sqrt{(\langle s^2 \rangle - \langle s \rangle^2)/M}}{\langle s \rangle} = \frac{\sqrt{1 - \langle s \rangle^2}}{\sqrt{M} \langle s \rangle} \propto \frac{e^{\beta N_p \Delta f}}{\sqrt{M}}, \quad (1.19)$$

and similarly for the numerator of Eq. (1.18).

Auxiliary field, or determinant QMC can also be formulated to probe ground state properties, and a sign problem arises similarly. In fact, this problem plagues all QMC methods, even though we showed it only for the determinant method⁹. The latter is the most robust, unbiased, and reliable method, with a generally modest sign problem, hence we choose it to carry out our simulations.

Furthermore, in general, it suffices to use the finite temperature auxiliary field method with β large enough to probe ground state properties (for example, this is shown numerically for the Hubbard model in the square lattice in [57]). In this case, the inverse temperature may be regarded as being analogous to a projective parameter Θ , characterizing convergence to the ground state, within statistical uncertainty. Projector QMC, the zero temperature version of auxiliary field QMC is based on an equation similar to Eq. (1.16). Any observable A is computed by use of a trial wave function with

⁸Although, there is a finite number of field configurations, the number grows exponentially with the number of sites on the lattice.

⁹So called because, as we shall show later, p_c boils down to a product of determinants that depends on the energy scales of the problem.

some overlap with the ground state $\langle \psi_T | \psi_0 \rangle \neq 0$ (see [58] for more details on the projector method; in this work we focus on the finite temperature version since it is more general):

$$\langle A \rangle = \lim_{\Theta \rightarrow \infty} \frac{\langle \psi_T | e^{-\Theta \mathcal{H}} A e^{-\Theta \mathcal{H}} | \psi_T \rangle}{\langle \psi_T | e^{-2\Theta \mathcal{H}} | \psi_T \rangle} \quad (1.20)$$

Note that auxiliary field QMC is more powerful than the variational and diffusion methods outlined before since it requires much less *a priori* information about the system. Perhaps more importantly, recent work suggests that it can be used in conjunction with neural networks to discover quantum phase transitions in correlated systems [59] in what could be a revolution in the field.

1.5 Original Contributions

In this work we focus mainly on the study of the magnetic properties of TMD nanoribbons. To carry out this study, we use our own original implementation of the auxiliary field QMC algorithm in C++. To validate the built software, we consider previously well known models (such as the Hubbard model on the 1D chain, and the square lattice), and compare our QMC results with those obtained in the mean field approximation and benchmark them against existing, “tried and true” implementations (namely ALF [60] and QUEST [61]), and early seminal studies [4, 57].

The code we wrote can be used to simulate low-dimensional Hubbard-like models with different geometries to extend this work further. Additionally, using our code, we characterize and compare different options to stabilize the matrix products needed to perform the simulations, and characterize the fermion sign problem. This last step is needed to extract the maximum amount of information out of the Monte Carlo measurements, since the fermion sign problem may become relevant for specific combinations of parameters of a given model.

To study TMD nanoribbons, we extend a minimal three-band tight binding model [50] to the interacting case. Then, we characterize TMD nanoribbons via original mean field and QMC calculations, which we compare as we did in the software validating phase.

1.6 Outline

We started this introductory chapter with the concept of emergence in strongly correlated electron systems. Then, we proceeded to discuss the particular example we study in this thesis: the 2D TMD nanoribbon. In this system, electron correlations give rise to interesting forms of magnetism, which, as far as we know, were unexplored numerically before this work. To tackle this interacting fermion system, we resort to a state-of-the-art QMC algorithm.

In chapter (2), we introduce the Hubbard model, a ubiquitous model of electron correlations. We discuss analytical solutions of simple limiting cases, outline some approximation methods, and introduce Green’s functions, which turn out to be the main object of our simulations. Moreover, we formulate the mean field theory of the Hubbard model.

Then, we proceed to the simulation method. In chapter (3), we start by summarizing the main

ideas about how to apply the Monte Carlo method to statistical physics problems. In this context, we use original results of our simulations to illustrate the concepts in the specific context of our problem. Still in chapter (3), we introduce the auxiliary field method, and its various challenges, namely low temperature, and large size stabilization, and the fermion sign problem.

In chapter (4), we apply the code we implemented for a variety of systems, benchmarking our code, and carrying out some original calculations.

Finally, in chapter (5), we conclude by discussing the results obtained in the previous chapter in the context of the literature, and propose future work to be done on the topic.

2

Minimal models of electron correlations in energy bands

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The interactions between the electrons in a solid give rise to effects that arise specifically due to the many-body nature of the system. The Hubbard model is a minimal model that encapsulates electron correlations. It goes beyond the periodic ionic potential perturbation to the free electron gas or tight binding approaches, which lead to band theory. One obtains the Hubbard Hamiltonian by adding the simplest possible electron-electron interaction term to a tight binding Hamiltonian: an on-site interaction term that penalizes double occupancy. From it, we can make predictions about properties of a strongly correlated system, namely magnetic and superconducting behavior, and metal-insulator transitions. We start with an overview of the Hubbard model and in the following chapters we provide details on how to simulate it numerically using Quantum Monte Carlo. We discuss the original motivation provided by Hubbard to introduce the model and show how its Hamiltonian arises as an approximate representation of the Coulomb repulsion between electrons in an energy band. Then, we present exact solutions for particular limiting cases, which will be used to crosscheck our simulations. In particular, we show that, in the limit where the interaction is large, the effective Hamiltonian at half filling corresponds to an atomic Heisenberg model defined in the appropriate Hilbert space with one electron per site. Then, we introduce Green's functions and explain how they relate to Wick's theorem. We proceed by formulating the mean field theory of the Hubbard model, and comparing results for a 1D chain with those obtained from Stoner's criterion. Finally, we show how one can generalize the Hubbard Hamiltonian and finish by discussing what type of interaction terms may be recast in a way that is more prone to simulation by writing the problem in terms of free fermions interacting with an external field.

2.1 Modelling electron correlations

The Hubbard model appeared in 1963 as one of the first attempts to include electron interaction effects in a quantum mechanical description of a solid. Originally, it was introduced to explain the behavior of the electrons in the narrow, partially filled d -bands of transition metals [32]. Correlation phenomena due to the Coulomb repulsion between the electrons in these bands lead to a behavior reminiscent of the atomic picture of a solid. In fact, the model may simply be regarded as a minimal model of interacting electrons in an energy band of a solid, where only on-site interactions are considered. We have come a long way since the introduction of the Hubbard model and it is now arguably as paradigm-defining in many-body theory as the Ising model in statistical physics [62–64].

Although the Hubbard model was initially applied to transition metal monoxides like FeO, NiO, and CoO, which are antiferromagnetic insulators (and not metallic, as was initially thought)¹, it is a minimal model giving insight on insulating, magnetic, and even superconducting phases arising due to the effect of electron interactions in a variety of quantum systems.

¹They were predicted to be metals by band theory until they were found not to behave like metals empirically.

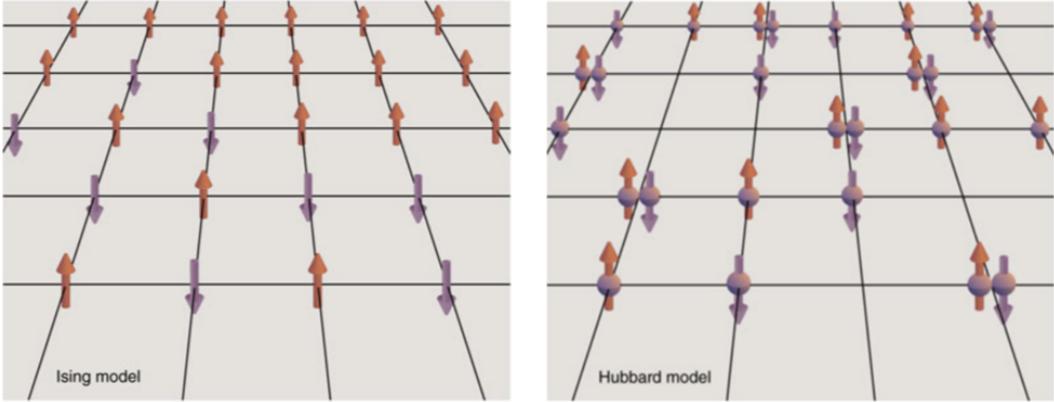


Figure 2.1: Unlike the Ising model, where either an up or a down spin live at each site, in the Hubbard model, there are four possible states at each site: a "hole" (absence of an electron), either an up spin electron or a down spin electron, or two electrons of opposite spins. The idea behind the model is to consider that the electrons interact, repelling each other, only when they are on the same site (taken from [65]).

Of course, Fig. (2.1) is only a simplified view presented for the sake of analogy. The Hubbard model is actually defined in terms of a Hamiltonian acting on electron wave functions centered in the sites of a lattice. Ultimately, we wish to determine, or at least approximate, the wave function describing the full electronic system. To do so, we must consider a Hamiltonian that allows simultaneous charge and spin fluctuations. It turns out that the wave function we seek is not, in general, a simple combination of products of one electron wave functions (a Slater determinant), as in the interaction-free case.

When Hubbard's seminal paper came out, it followed a trend that arose in the 1950's when people were working on a theory of correlation effects in the free electron gas [66–71]. Hubbard devised a simple model for the (at the time) seemingly intractable problem of interacting electrons in a band. His work explained qualitatively some properties of compounds containing transition metals, in which electron correlations are non negligible. It turns out that the mathematical formulation of the interaction problem for correlated electrons in a band is not prohibitively complicated, and is relatively amenable to both analytical and numerical computations after some controlled approximations are introduced. Notably, the model is particularly adapted to computer simulations because of the simple form of its Hamiltonian. Moreover, it has been shown to be very relevant in the description of Mott insulators, and high T_c superconductors². In fact, the Hubbard model has found many applications, describing successfully a variety of quantum systems [72]; nonetheless, even the simplified picture it offers is in general difficult to approach analytically. There exists an exact, albeit not very transparent solution in one dimension via Bethe ansatz [31], however the more general higher dimensional case is often solved numerically. An example of particular relevance for this work is the study carried out by Hirsch [7]. In the following chapters, we will discuss how to simulate the Hubbard model using a numerical approach that is based on this seminal paper, and essentially follows the ideas introduced in it.

²In this context, T_c is the critical temperature associated with the transition to a superconducting phase.

2.2 Hubbard model

The nearly free electron gas models the conduction bands of metals and alloys fairly accurately. The high mobility of the electrons compared to the ions justifies two equivalent approximations, both giving essentially the same results [73]. The first idea is to treat the periodic potential created by the *virtually* fixed ions (compared to the electrons) as a perturbation on the free electron gas. Equivalently, we may imagine the system as a collection of tightly bond atoms, in which the electrons in the higher energy band hop from atom to atom. Both these approaches lead to band theory, a framework which allows us to predict whether a material is a conductor or a insulator. From the tight binding point of view, the effect of the electron mobility is the broadening of the atomic energy levels: the electrons in the solid occupy energy bands, rather than levels. The partially filled band of highest energy is called the conduction band, since it is the band occupied by conduction electrons hopping from atom to atom. However, in transition metal and rare-earths, as in some compounds containing these elements, apart from the conduction bands there are partially filled bands: d - or f -bands. The partial filling of these bands and the electron correlations within them are responsible for the characteristic properties of these solids. Some of these properties are not explained by band theory, namely the Mott metal-insulator transition [74–76].

2.2.1 Electron correlations in narrow d -bands

First, note that the effects of correlations cannot possibly be the same in narrow energy bands and in the free electron gas. To see this, we may simply recall the shape of a d -wave function.

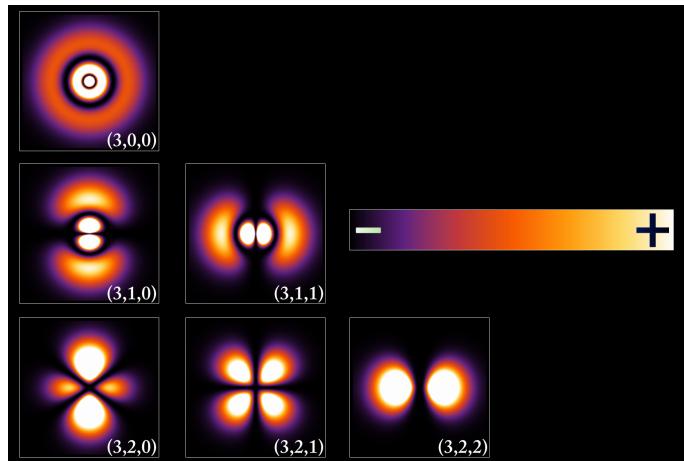


Figure 2.2: Probability density plots for different hydrogen orbital wave functions corresponding to quantum numbers (n, l, m) for $n = 3$. d -wave functions correspond to $l = 2$. Note that the probability density is always higher in a region near the nucleus, and has a complicated shape, which will lead to a non-uniform distribution of electronic charge, as opposed to the case of the free electron gas. (adapted from [77])

In a d -orbital, the electron charge density is concentrated near the nucleus. In a solid, the electronic charge density should then also be concentrated near the nuclei, as long as the atomic description is useful, even if not completely correct³. It is much smaller between atoms so that electrons do seem to

³The electronic charge density is, of course, not actually defined in terms of a squared norm of the d -wave function for a narrow band. There is some broadening of the corresponding atomic energy level, and the wave function describing

belong to individual atoms in some sense. For a d -band, we assume this description to hold to some extent since the band is narrow. Thus, the fact that we may speak with some meaning of an electron belonging to a particular atom motivates a description from which the atomic characteristics of the solid emerge, in spite of the fact that the bandwidth of a d -band is still appreciable. The point is that electrons in d -bands are certainly not well described by a free electron gas, which cannot possibly account for atomic-like behavior.

Experimentally, d -electrons of transition metals show hybrid behavior: sometimes they are accurately described by an ordinary band model, but there are occasions in which the atomic model is better. For example, we see spin wave phenomena in ferromagnetic transition metals, and the susceptibilities of some of these metals depend strongly on temperature. This is characteristic of an atomic (Heisenberg) model. On the other hand, the d -electrons contribute significantly to the low temperature specific heat and sometimes the magnetic moments per atom of some transition metal ferromagnets are not integer multiples of the Bohr magneton. This is characteristic of band theory⁴. Our theory of correlations should describe this balance between band-like and atomic-like behavior.

The atomic picture of a solid consists of an electron gas where ions are immersed. The ions then interact in much the same way as they do in salts. This extreme scenario is surely not even close to the true state of affairs since the number of d -electrons per atom is in general not an integer. This motivates us to introduce a less restrictive model, which is not too far from the atomic model. We shall assume that while d -electrons still have some band motion, they are strongly correlated with each other so that the solid retains some atomic-like behavior. The correlations between electrons on different atoms are likely much weaker and we neglect them.

Let us now look at an example of the aforementioned circumstance. Take a partially filled d -band of non-interacting electrons. The spin of any given atom in the solid is just the total spin of all electrons on that atom. It fluctuates both in magnitude and in direction, with a characteristic time that depends on how frequently d -electrons hop. We can estimate the time interval between d -electron hopping events between atoms as being of the order \hbar/Δ , where Δ is the d -electron bandwidth. The spin can thus be thought of as being associated to each individual (and constantly hopping) d -electron.

How do the electron interactions affect this picture? We start by recalling Hund's rule: the nature of the interactions between atoms leads to an alignment of the spins on each atom. Since the atomic picture seems to prevail in our metal, we have reason to expect a similar effect to occur. An atom with a total spin in some direction at a given time will tend to attract electrons with the spin on that direction and repel those with opposite spin. This mechanism makes it unlikely for the spin of an atom to change much over time. If the interactions between atoms are strong enough, the correlations become considerable and, making our statement more precise, the total spin of an atom will persist for

an electron is a Bloch wave function. Since the band is narrow, we assume that the atomic wave function description is still somewhat useful in a given range and we use it to provide a heuristic motivation for the non validity of the free electron assumption.

⁴Think, for example, of a tight binding model. Electrons hop from atom to atom, and in general the spin of each atom depends on the particular electrons "belonging" to it at a given time. If we take an average of the total spin of each atom, we will in general not necessarily obtain an integer multiple of the Bohr magneton. If we simply had a collection of atoms, Hund's rule would apply, and each atom would have its spin aligned in a given direction. The average spin would then tend to be an integer multiple of the Bohr magneton.

a time that is long compared with the d -electron hopping time. Note that it is not the localization of the electrons that causes the spin state of the atom to persist. The specific electrons belonging to a given atom change all the time as long as their spin is consistent with the total spin requirement imposed by Hund's rule. For strong enough correlations, we may think of the spin as being associated to each atom, which opens up the possibility to describe the system using an atomic (Heisenberg) model, as we shall see later.

A theory of electron correlations in a narrow energy band should reduce to an atomic model in the appropriate limit, for example atoms that are so far apart on a lattice that they interact only very weakly. Although we always keep in mind that we are focusing on d -electrons, we shall consider s -electrons in what follows for the sake of simplicity. The important conclusions will not differ significantly. We will use the "atomicity" of the electronic distribution to introduce an approximate representation of the electron interaction. It turns out that this representation is mathematically much simpler to handle than the Coulomb interaction itself.

In short, our picture is the following: electrons hop rapidly from atom to atom in a band-like fashion, but their motion is correlated in such a way that atomic characteristics emerge. The extent of atomic behavior depends, of course, on the strength of the interaction.

2.2.2 Hubbard Hamiltonian

Imagine a hypothetical partially filled narrow s -band with n electrons per atom. Suppose you have obtained Bloch wave functions $\psi_{\mathbf{k}}$ corresponding to energies $\varepsilon_{\mathbf{k}}$ by solving the Schrödinger equation for some spin-independent Hartree-Fock potential that accounts for the average interaction of the s -band electrons with electrons on other bands, and the interaction with the other s -electrons. The electrons on the band evolve according to the Hamiltonian:

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \left(\varepsilon_{\mathbf{k}} - \sum_{\mathbf{k}'} (2V_{\mathbf{k}\mathbf{k}'}^{\mathbf{k}\mathbf{k}'} - V_{\mathbf{k}'\mathbf{k}'}^{\mathbf{k}\mathbf{k}'}) \nu_{\mathbf{k}'} \right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \mathbf{k}' \mathbf{k}' \sigma_1 \sigma_2}} V_{\mathbf{k}'_1 \mathbf{k}'_2}^{\mathbf{k}_1 \mathbf{k}_2} c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_2 \sigma_2} c_{\mathbf{k}'_1 \sigma_1}, \quad (2.1)$$

where the \mathbf{k} -sums run over the first Brillouin zone.

The integrals are defined by

$$V_{\mathbf{k}'_1 \mathbf{k}'_2}^{\mathbf{k}_1 \mathbf{k}_2} \equiv \left\langle \mathbf{k}_1 \mathbf{k}_2 \left| \frac{e^2}{r} \right| \mathbf{k}'_1 \mathbf{k}'_2 \right\rangle = e^2 \int \frac{\psi_{\mathbf{k}_1}^*(\mathbf{x}) \psi_{\mathbf{k}'_1}(\mathbf{x}) \psi_{\mathbf{k}_2}^*(\mathbf{x}') \psi_{\mathbf{k}'_2}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d\mathbf{x} d\mathbf{x}' \quad (2.2)$$

The first term represents the band energies of the electrons minus their potential energy in the part of the Hartree-Fock field due to the electrons of the s -band itself. The latter ensures that we do not overestimate the magnitude of the interactions between the electrons of the band: the Hartree-Fock field that specifies $\varepsilon_{\mathbf{k}}$ is computed taking into account these interactions, so if we didn't subtract it, we would count the energy of these interactions twice since they reappear in the last term, which represents the interactions among all electrons in the system. Furthermore, we assume that up and down spins are occupied equally, and $\nu_{\mathbf{k}}$ are the occupation numbers of the states of the band in the

Hartree-Fock calculation.

The term that we subtract in equation (2.1) corresponds to the part of the interaction term which is already accounted for by the first diagonal “mean field” term. Thus, it corresponds to the mean field expansion of the interaction term. A generic way of writing the interaction term by gathering the \mathbf{k}, σ indexes into a single index μ is

$$V_{\text{int}} = \frac{1}{2} V_{\nu' \mu'}^{\nu \mu} c_{\nu}^{\dagger} c_{\mu}^{\dagger} c_{\mu'} c_{\nu'}, \quad (2.3)$$

where the summation over repeated indexes is implied. In appendix A, we obtain the mean field form of V_{int} in the Hartree-Fock approximation.

Now consider the Wannier functions

$$\phi(\mathbf{x}) = N^{-1/2} \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}), \quad (2.4)$$

where N is the number of atoms. We may write $\psi_{\mathbf{k}}$ as a combination of Wannier functions localized at each atom.

$$\psi_{\mathbf{k}}(\mathbf{x}) = N^{-1/2} \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi(\mathbf{x} - \mathbf{R}_i), \quad (2.5)$$

where the sum runs over all atomic positions \mathbf{R}_i . Introducing the annihilation (creation) operators of an electron of spin σ in the Wannier state $\phi(\mathbf{x} - \mathbf{R}_i)$ localized at site i , $c_{i\sigma}^{(\dagger)}$, we may write

$$c_{\mathbf{k}\sigma}^{(\dagger)} = N^{-1/2} \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} c_{i\sigma}^{(\dagger)} \quad (2.6)$$

Thus, the Hamiltonian becomes

$$\mathcal{H} = \sum_{ij} K_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{ijkl} \left[\frac{1}{2} V_{kl}^{ij} c_{i\sigma}^{\dagger} c_{j\sigma}^{\dagger} c_{l\sigma'} c_{k\sigma} - \left(2V_{kl}^{ij} - V_{lk}^{ij} \right) \nu_{jl} c_{i\sigma}^{\dagger} c_{k\sigma} \right], \quad (2.7)$$

where

$$K_{ij} = N^{-1} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}, \text{ and } \nu_{jl} = N^{-1} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_l)} \quad (2.8)$$

Now comes the crucial approximation. For a narrow energy band, the Wannier functions ϕ nearly coincide with atomic s -functions. For small bandwidth, these s -functions form an atomic shell whose radius is small compared with the spacing between atoms, that is, the lattice constant. Thus, the integral $U = \langle ii | e^2/r | ii \rangle$ should turn out to be much larger than all other integrals. This suggests the seemingly crude approximation of neglecting all other integrals. However, this approximation is not so radical as it could seem at first sight since the other integrals are indeed much smaller than U . In fact, for example, for $3d$ electrons of transition metals they are smaller by about two orders of magnitude [32]. Keeping only the terms in U in the interaction part, we obtain

$$\mathcal{H} = \sum_{i,j,\sigma} K_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i,-\sigma} - U \sum_{i,\sigma} \nu_{i,i} n_{i,\sigma} \quad (2.9)$$

where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. Note that $\nu_{i,i} = N^{-1} \sum_{\mathbf{k}} \nu_{\mathbf{k}} = n/2$, where n is the electron density, which means that the last term is constant and may be dropped. Now, the hopping matrix \mathbf{K} can, in principle, be found by inverse Fourier transforming the dispersion relation $\varepsilon_{\mathbf{k}}$ of the equivalent interaction-free system, that we can assumed to be obtained experimentally or numerically. In the purely tight binding view (with no U -term), we have a well defined crystal wavevectors that depends on the symmetry of the lattice, which may be written as Fourier transforms

$$|\mathbf{k}\rangle \equiv \frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle \quad (2.10)$$

Recalling the form of the hopping Hamiltonian (or the kinetic energy part in the Hubbard model)

$$\mathcal{H}_K = - \sum_{\mathbf{r}\mathbf{r}'} K(\mathbf{r} - \mathbf{r}') |\mathbf{r}'\rangle \langle \mathbf{r}| \quad (2.11)$$

we can obtain the dispersion relation.

$$-\mathcal{H}_K |\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}\mathbf{r}'} K(\mathbf{r} - \mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}'\rangle = \frac{1}{\sqrt{N}} \left(\sum_{\mathbf{R}} K(\mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{R}} \right) \left(\sum_{\mathbf{r}'} e^{i\mathbf{k}\cdot\mathbf{r}'} |\mathbf{r}'\rangle \right) = \varepsilon_{\mathbf{k}} |\mathbf{k}\rangle \quad (2.12)$$

and here we recognize the dispersion relation as the (negative) Fourier transform of the hopping

$$\varepsilon_{\mathbf{k}} = - \sum_{\mathbf{R}} K(\mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{R}} \quad (2.13)$$

This gives us an interpretation of the \mathbf{K} matrix: given the dispersion relation, and considering the solid to be well described by a tight binding model, we can easily obtain the matrix elements K_{ij} .

Let us now suppose that we have the simplest uniform nearest neighbor hopping model. Going back to equation (2.8), and recalling that the sum on \mathbf{k} is restricted to the first Brillouin zone, we obtain the usual tight binding result: $K_{\langle ij \rangle} = -t \in \mathbb{R}$ and 0 otherwise (i.e. \mathbf{K} is a very sparse matrix that is only non-zero for i, j nearest neighbors). The Hubbard Hamiltonian is then

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_i \left(n_{i,\uparrow} + n_{i,\downarrow} \right), \quad (2.14)$$

where, for generality, we included an arbitrary chemical potential, so that we use the Grand-canonical ensemble (GCE).

2.2.3 Particle-hole symmetry

In this section we examine a particularly relevant and unique symmetry of the Hubbard model. The main idea is that, at half filling, the Hubbard Hamiltonian is invariant under a transformation which turns particles into holes and vice-versa. Particle-hole symmetry (PHS) allows us to relate the

properties of the Hubbard Hamiltonian at different values of the parameters. Moreover, it allows us to devise a mapping between the attractive ($U < 0$) and the repulsive ($U > 0$) models. We will see later that this mapping is important in QMC simulations [78].

We start our discussion with the concept of a bipartite lattice. A lattice is said to be bipartite if it can be divided into two sublattices \mathcal{A} and \mathcal{B} , such that the set of neighbors of a site in sublattice \mathcal{A} belongs to sublattice \mathcal{B} . For example, the square and honeycomb lattices are bipartite, whereas the triangular lattice is not. In a bipartite lattice, Antiferromagnetic (AF) order is favored. In contrast, AF order is frustrated on the triangular and other non bipartite lattices.

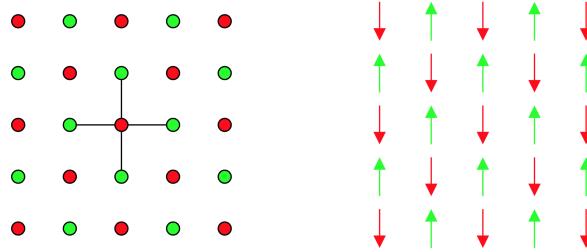


Figure 2.3: On the left, we see that the square lattice is bipartite. The neighbors of a particular site in the red sublattice all belong to the green sublattice. The picture on the right is meant to give some intuition on why the bipartite lattice favors AF order. We represent a configuration where fermions of a given spin have as their neighbors only fermions of opposite spin, which would be favored by Heisenberg exchange (taken from [78]).

Introducing a Particle-hole transformation (PHT),

$$d_{i,\sigma}^\dagger = (-1)^i c_{i,\sigma}, \quad (2.15)$$

we exchange the role of annihilation and creation operators. In fact, particles become holes and vice-versa: $d_{i,\sigma}^\dagger d_{i,\sigma} = 1 - c_{i,\sigma}^\dagger c_{i,\sigma}$, and the occupations $n = 0, 1$ are interchanged. Consider a bipartite lattice. Since in that case the factor $(-1)^i$ takes on -1 on one sublattice and 1 on the other, the kinetic part of the Hamiltonian is invariant under a PHT:

$$c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \mapsto (-1)^{i+j} (d_{i,\sigma}^\dagger d_{j,\sigma}^\dagger + d_{j,\sigma}^\dagger d_{i,\sigma}^\dagger) = d_{j,\sigma}^\dagger d_{i,\sigma} + d_{i,\sigma}^\dagger d_{j,\sigma} \quad (2.16)$$

The PHS form of the kinetic term can be incorporated into the interaction term by a shift in the chemical potential and by adding a constant to the Hamiltonian. First, note that the term

$$U \left(n_{i,\uparrow} - \frac{1}{2} \right) \left(n_{i,\downarrow} - \frac{1}{2} \right)$$

is unchanged under a PHT. Expanding this term, we obtain $U n_{i,\uparrow} n_{i,\downarrow} - \frac{U}{2} (n_{i,\uparrow} + n_{i,\downarrow}) + \frac{U}{4}$, which indeed differs from the original interaction term by a shift in the chemical potential ($\mu \rightarrow \mu + U/2$) plus a constant. Thus, the particle-hole symmetric form of the Hamiltonian

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{i,\sigma}^\dagger c_{j,\sigma} \right) + U \sum_i \left(n_{i,\uparrow} - \frac{1}{2} \right) \left(n_{i,\downarrow} - \frac{1}{2} \right) - \mu \sum_i \left(n_{i,\uparrow} + n_{i,\downarrow} \right) \quad (2.17)$$

is completely equivalent to the original Hamiltonian.

Under a PHT, the density, $\rho = \langle n_\uparrow + n_\downarrow \rangle$, transforms as $\rho \mapsto 2 - \rho$. The Hamiltonian changes only in the chemical potential term: $\mu \mapsto -\mu$. Thus, we have that $\rho(\mu) = 2 - \rho(-\mu)$, and at $\mu = 0$, we have half filling: $\rho = 1$. This reasoning is valid for any β , t , or U , which implies that the phase diagram of the Hubbard model must be symmetric about half filling. Suppose you added next nearest neighbor (NNN) hoppings t' ⁵. Then, PHS would be broken, and the phase diagram would no longer be symmetric about $\mu = 0$. Indeed, a modified version of the Hubbard model with NNN hoppings is often used to model cuprate superconductors, and this lack of symmetry is consistent with the fact that hole- and electron-doped cuprates have different properties. PHS is also broken for the triangular lattice with non uniform hoppings we shall consider later when modelling Transition Metal Dichalcogenides (TMDs).

2.3 Exact solutions for simple cases

In PHS form, the Hubbard Hamiltonian may then be written as a sum of kinetic and chemical, and potential energy terms $\mathcal{H} = \mathcal{H}_K + \mathcal{H}_V$, defined as

$$\mathcal{H}_K = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) - \mu \sum_i \left(n_{i,\uparrow} + n_{i,\downarrow} \right), \quad \mathcal{H}_V = U \sum_i \left(n_{i,\uparrow} - \frac{1}{2} \right) \left(n_{i,\downarrow} - \frac{1}{2} \right), \quad (2.18)$$

where i and j label sites on the lattice; $c_{i,\sigma}^\dagger$ is an operator that annihilates (creates) an electron with spin σ on site i ; $n_{i,\sigma}$ is the number operator counting the number of electrons of spin σ on site i (either 0 or 1); t is the hopping parameter related to the kinetic energy of the electrons: it is determined by the overlap of the atomic wave functions on neighboring sites $\langle i,j \rangle$; U is the on-site Coulomb repulsion between electrons: whenever a site i has two electrons, there is a local repulsion between them corresponding to an energy cost $Un_{i,\uparrow}n_{i,\downarrow}$ (up to an additive constant); μ is the chemical potential controlling the electron number (or density).

A given physical observable of interest \mathcal{O} , such as the spin-spin correlation, or the magnetic susceptibility may be computed formally by

$$\langle \mathcal{O} \rangle = \text{Tr}[\mathcal{O}\mathcal{P}] \quad (2.19)$$

where

$$\mathcal{P} \equiv \frac{1}{Z} e^{-\beta \mathcal{H}}, \quad \text{with } Z = \text{Tr}[e^{-\beta \mathcal{H}}] \quad (2.20)$$

The trace is taken over the Hilbert space corresponding to all possible configurations of the lattice occupation. Defining an orthonormal basis of this Hilbert space $\{|\psi_\alpha\rangle | \alpha = 1, \dots, D\}$, where D is the dimension of the Hilbert space, the partition function reads

⁵On the square lattice, this corresponds to connecting sites across the diagonal of each square.

$$\text{Tr}[e^{-\beta \mathcal{H}}] = \sum_{\alpha} \langle \psi_{\alpha} | e^{-\beta \mathcal{H}} | \psi_{\alpha} \rangle \quad (2.21)$$

There are four possible states at each site in the Hubbard model: $| \rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$, corresponding, respectively, to no electron, a spin up or spin down electron, and two electrons of opposite spin occupying the site. The potential energy operator acts as follows

$$U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \begin{cases} | \rangle = \frac{U}{4} | \rangle \\ |\uparrow\rangle = -\frac{U}{4} |\uparrow\rangle \\ |\downarrow\rangle = -\frac{U}{4} |\downarrow\rangle \\ |\uparrow\downarrow\rangle = \frac{U}{4} |\uparrow\downarrow\rangle \end{cases} \quad (2.22)$$

Singly occupied states ($|\uparrow\rangle$, $|\downarrow\rangle$) have lower energy and are thus more likely to occur. They correspond to nonzero magnetization $m = n_{\uparrow} - n_{\downarrow}$, which is favored by the Hubbard interaction U . A relevant question is whether or not the spins order in space when $t \neq 0$ and to what extent.

Let us now establish our notations for second quantized operators to introduce a different representation of electronic states on the lattice. The fermionic annihilation and creation operators anticommute: $\{c_{j\sigma}, c_{l\sigma'}^{\dagger}\} = \delta_{jl}\delta_{\sigma\sigma'}$. The c -operator algebra is further defined by the vanishing of all other anticommutators: $\{c_{j\sigma}^{(\dagger)}, c_{l\sigma'}^{(\dagger)}\} = 0$. Note that taking $l = j$ and $\sigma = \sigma'$ in this equation for the c^{\dagger} -operators, we recover Pauli's exclusion principle since $(c_{j\sigma}^{\dagger})^2 = 0$. If we omit the site i and spin σ indices, a convenient way of specifying states on the lattice is

$$|0\rangle : \text{unoccupied state - no electron} \quad |1\rangle : \text{occupied state - one electron} \quad (2.23)$$

so that a generic state may be written as a product of the states above $\otimes_{i=1}^N \otimes_{\sigma=\pm 1/2} |n\rangle_{i,\sigma}$ at each site for each spin state, where $n = 0, 1$. For example, one such state is

$$|0\rangle_{1,\uparrow} |1\rangle_{1,\downarrow} |1\rangle_{2,\uparrow} |1\rangle_{2,\downarrow} |0\rangle_{3,\uparrow} |0\rangle_{3,\downarrow} \dots |1\rangle_{N,\uparrow} |0\rangle_{N,\downarrow}, \quad (2.24)$$

where N is the number of sites on the lattice. Site 1 has a single spin-down electron, while site 2 is doubly occupied, site 3 is unoccupied, and so on, until we reach site N , which has a single spin-up electron. The creation and annihilation operators act as follows

$$c|0\rangle = 0 \quad c^{\dagger}|0\rangle = |1\rangle \quad c|1\rangle = |0\rangle \quad c^{\dagger}|1\rangle = 0 \quad (2.25)$$

Thus, the eigenstates of the number operator are $|0\rangle, |1\rangle$: $n|0\rangle = 0, n|1\rangle = |1\rangle$. Moreover, the operator $c_i^{\dagger}c_{i+1}^{\dagger}$, corresponding to the hopping from site $i + 1$ to i , i.e. to the kinetic energy of the electrons on neighboring sites, annihilates the particle at $i + 1$ and creates it back at i , i.e. the electron hops from $i + 1$ to i . Ignoring spin:

$$c_i^\dagger c_{i+1}^\dagger \begin{cases} |00\rangle = 0 \\ |10\rangle = 0 \\ |01\rangle = |10\rangle \\ |11\rangle = c_i^\dagger |10\rangle = 0 \end{cases} \quad (2.26)$$

2.3.1 The purely atomic ($\frac{U}{t} \rightarrow \infty$), single site limit

When $t = 0$, the site index may be omitted since the Hamiltonian is a sum of operators solely at site i . Hence, we have $[\mathcal{H}, n_{i,\sigma}] = 0 \forall i = 1, 2, \dots, N$, and the eigenstates of \mathcal{H} are also eigenstates of all number operators at the different sites in the lattice. Thus, in the single site limit, we obtain

$$\mathcal{H} = U \left(n_\uparrow - \frac{1}{2} \right) \left(n_\downarrow - \frac{1}{2} \right) - \mu (n_\uparrow + n_\downarrow) \quad (2.27)$$

which acts as follows (using the eigenstates of n_σ)

$$\mathcal{H} \begin{cases} | \rangle = \frac{U}{4} | \rangle \\ |\uparrow\rangle = \left(\frac{U}{4} - (\mu + \frac{U}{2}) \right) |\uparrow\rangle \\ |\downarrow\rangle = \left(\frac{U}{4} - (\mu + \frac{U}{2}) \right) |\downarrow\rangle \\ |\uparrow\downarrow\rangle = \left(\frac{U}{4} - 2\mu \right) |\uparrow\downarrow\rangle \end{cases} \quad (2.28)$$

Thus, the Hamiltonian is diagonal in the basis $\{|\psi_\alpha\rangle\} = | \rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$:

$$\mathcal{H} \rightsquigarrow \mathbf{H} = \text{diag} \left(\frac{U}{4}, \frac{U}{4} - (\mu + \frac{U}{2}), \frac{U}{4} - (\mu + \frac{U}{2}), \frac{U}{4} - 2\mu \right), \quad (2.29)$$

which means that $e^{-\beta\mathcal{H}}$ is also diagonal:

$$e^{-\beta\mathcal{H}} \rightsquigarrow e^{-\beta U/4} \text{diag} \left(1, e^{\beta(\mu+\frac{U}{2})}, e^{\beta(\mu+\frac{U}{2})}, e^{2\beta\mu} \right) \quad (2.30)$$

and this is one of the rare situations in which it is possible to explicitly write down a closed form for the partition function.

$$Z = \text{Tr}[e^{-\beta\mathcal{H}}] = \sum_\alpha \langle \psi_\alpha | e^{-\beta\mathcal{H}} | \psi_\alpha \rangle = e^{-\beta U/4} \left(1 + 2e^{\beta(\mu+\frac{U}{2})} + e^{2\beta\mu} \right) \quad (2.31)$$

Moreover, some of the observables that were mentioned before are explicitly computable. This is because due to the diagonal form of \mathcal{H} , the expressions defining these observables greatly simplify.

$$\begin{aligned}
\mathcal{H}e^{-\beta\mathcal{H}} &\rightsquigarrow e^{-\beta U/4} \text{diag}\left(\frac{U}{4}, (-\mu - \frac{U}{4})e^{\beta(\mu + \frac{U}{2})}, (-\mu - \frac{U}{4})e^{\beta(\mu + \frac{U}{2})}, (\frac{U}{4} - 2\mu)e^{2\beta\mu}\right) \\
n_{\uparrow}e^{-\beta\mathcal{H}} &\rightsquigarrow e^{-\beta U/4} \text{diag}\left(0, e^{\beta(\mu + \frac{U}{2})}, 0, e^{2\beta\mu}\right) \\
n_{\downarrow}e^{-\beta\mathcal{H}} &\rightsquigarrow e^{-\beta U/4} \text{diag}\left(0, 0, e^{\beta(\mu + \frac{U}{2})}, e^{2\beta\mu}\right) \\
n_{\uparrow}n_{\downarrow}e^{-\beta\mathcal{H}} &\rightsquigarrow e^{-\beta U/4} \text{diag}\left(0, 0, 0, e^{2\beta\mu}\right)
\end{aligned} \tag{2.32}$$

From these we can compute some traces which we shall find useful to obtain averages of various observables.

$$\begin{aligned}
\text{Tr} \left[\mathcal{H}e^{-\beta\mathcal{H}} \right] &= e^{-\beta U/4} \left(\frac{U}{4} + 2(-\mu - \frac{U}{4})e^{\beta(\mu + \frac{U}{2})} + (\frac{U}{4} - 2\mu)e^{2\beta\mu} \right) \\
\text{Tr} \left[(n_{\uparrow} + n_{\downarrow})e^{-\beta\mathcal{H}} \right] &= e^{-\beta U/4} \left(2(-\mu - \frac{U}{4})e^{\beta(\mu + \frac{U}{2})} + (\frac{U}{4} - 2\mu)e^{2\beta\mu} \right) \\
\text{Tr} \left[n_{\uparrow}n_{\downarrow} \right] &= e^{-\beta U/4} e^{2\beta\mu}
\end{aligned} \tag{2.33}$$

The bottom line is that we are able to obtain *exact* expressions for

1. the one-site density $\rho = \langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle$, measuring the average occupation of each site.

$$\rho = \frac{\text{Tr}[(n_{\uparrow} + n_{\downarrow})e^{-\beta\mathcal{H}}]}{Z} = \frac{2e^{\beta(\frac{U}{2} + \mu)} + 2e^{2\beta\mu}}{1 + 2e^{\beta(\mu + \frac{U}{2})} + e^{2\beta\mu}} \tag{2.34}$$

Note that when there is no chemical potential $\mu = 0$, we have $\rho = 1$ for any U , or β . This corresponds to half filling: the density of electrons is half its maximum possible value.

In Fig. (2.4), we plot $\rho(\mu)$ for varying temperature, and fixed on-site interaction. It allows us to get some insight into the Mott insulating gap. At $T = 0.25$, the curve owes its step-like shape to the small thermal fluctuations. As T increases, the curve starts losing this tendency, and by $T = 2.0$, it is no longer possible to identify it. This is a consequence of the now larger thermal fluctuations that are present at higher temperature. We denote the flat region between $\mu = -U/2$ and $\mu = U/2$ “Mott Plateau”. As the chemical potential is increased, the density remains small until a threshold is exceeded at $\mu = -\frac{U}{2}$. Then, it rises very rapidly to $\rho = 1$ (half filling), and again stays almost constant. It is not until μ jumps by U that we fill the site ($\rho = 2$). This Mott insulating gap appears because the presence of a fermion in the site blocks the addition of a second one due to the on-site interaction. One needs a sufficiently large chemical potential to overcome this effect. As we shall see, this feature of the model remains present as the number of sites increases. Note that in the Mott gap, the compressibility vanishes: $\kappa = \frac{\partial \rho}{\partial \mu} = 0$, leading to the appearance of the Mott Plateau. Just as thermal fluctuations can destroy the sharp jumps corresponding to the gap, so can quantum fluctuations. The hopping term in the Hamiltonian introduces such fluctuations, leading to an effect similar to that of Fig. (2.4).

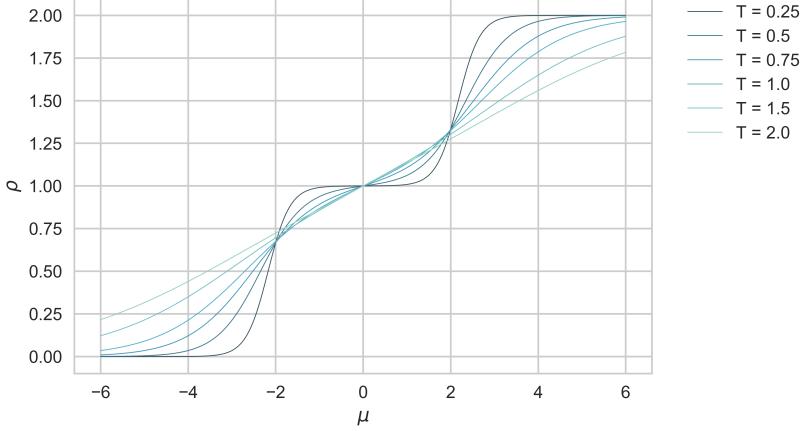


Figure 2.4: Electron density ρ for varying chemical potential μ and temperature $T = \beta^{-1}$, but fixed $U = 4$. As the temperature decreases, a “Mott plateau” sets in. The Mott insulating gap already seen here is an important feature of the Hubbard model.

2. the one-site energy $E = \langle \mathcal{H} \rangle$.

$$\begin{aligned}
E &= \frac{\text{Tr}\left(\mathcal{H}e^{-\beta\mathcal{H}}\right)}{Z} = \frac{\frac{U}{4} + 2(-\mu - \frac{U}{4})e^{\beta(\frac{U}{2}+\mu)} + (\frac{U}{4} - 2\mu)e^{2\beta\mu}}{1 + 2e^{\beta(\frac{U}{2}+\mu)} + e^{2\beta\mu}} \\
&= \frac{\frac{U}{4}(1 + 2e^{\beta(\frac{U}{2}+\mu)} + e^{2\beta\mu})}{1 + 2e^{\beta(\frac{U}{2}+\mu)} + e^{2\beta\mu}} + \frac{2(-\mu - \frac{U}{4})e^{\beta(\frac{U}{2}+\mu)} - 2\mu e^{2\beta\mu} - 2\frac{U}{4}e^{\beta(\frac{U}{2}+\mu)}}{1 + 2e^{\beta(\frac{U}{2}+\mu)} + e^{2\beta\mu}} \\
&= \frac{U}{4} - \frac{(2\mu - U)e^{\beta(\frac{U}{2}+\mu)} + 2\mu e^{2\beta\mu}}{1 + 2e^{\beta(\frac{U}{2}+\mu)} + e^{2\beta\mu}}
\end{aligned} \tag{2.35}$$

which at half filling becomes

$$E = \frac{U}{4} - \frac{U}{2(1 + e^{-\beta U/2})} \tag{2.36}$$

3. the double occupancy $\langle n_\uparrow n_\downarrow \rangle$.

$$\langle n_\uparrow n_\downarrow \rangle = \frac{\text{Tr}[n_\uparrow n_\downarrow]}{Z} = \frac{e^{2\beta\mu}}{1 + 2e^{\beta(\frac{U}{2}+\mu)} + e^{2\beta\mu}} \tag{2.37}$$

which, at half filling, simplifies to

$$\langle n_\uparrow n_\downarrow \rangle = \frac{1}{2(1 + e^{\beta U/2})} \tag{2.38}$$

Note that as either U or β increase the double occupancy tends to zero.

As was motivated in the previous chapter, we are interested in studying magnetism in correlated systems. For the Hubbard model, the relevant quantity is the local moment

$$\langle m^2 \rangle = \langle (n_\uparrow - n_\downarrow)^2 \rangle = \langle n_\uparrow - n_\downarrow \rangle - 2 \langle n_\uparrow n_\downarrow \rangle = \rho - 2 \langle n_\uparrow n_\downarrow \rangle \tag{2.39}$$

In Figs. (2.5, 2.6), we show how $\langle m^2 \rangle$ varies as a function of U for different temperatures, and how $\langle m^2 \rangle$ varies with T , for different values of the chemical potential, respectively. At low temperature

or for large on-site interaction, local moments tend to develop, which leads to magnetic ordering: $\langle m^2 \rangle \rightarrow 1$ (in the half-filled case). Since the double occupancy is zero in this case, if we do not consider thermal fluctuations, the magnetization corresponds to the spin of the electron occupying the site.

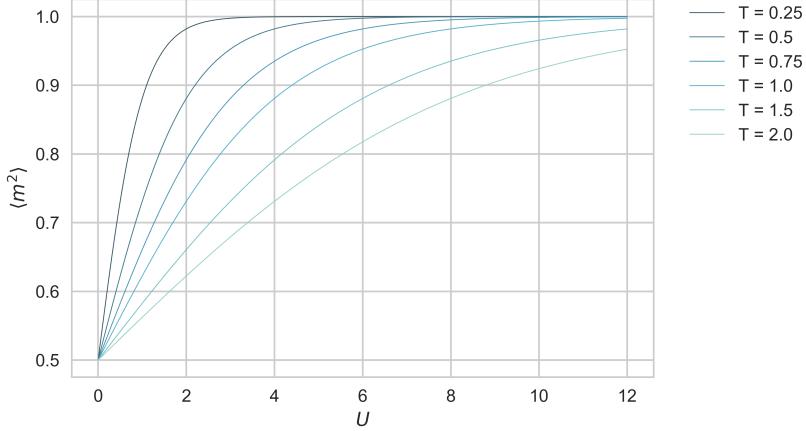


Figure 2.5: Magnetization as a function of the on-site interaction $\langle m^2 \rangle (U)$ in the single site Hubbard model for varying temperature T . Local moments are favored by the on-site interaction, and are more likely to develop at lower temperatures, when thermal fluctuations are smaller. Here we consider half filling: $\mu = 0$.

In Fig. (2.5), we see thermal fluctuations destroying magnetic ordering. As what happens for the Mott plateau, quantum fluctuations (i.e. introducing a hopping term in the Hamiltonian) change the behavior of the magnetization, and perfect moments ($\langle m^2 \rangle = 1$) do not form anymore at zero temperature for finite on-site interaction.

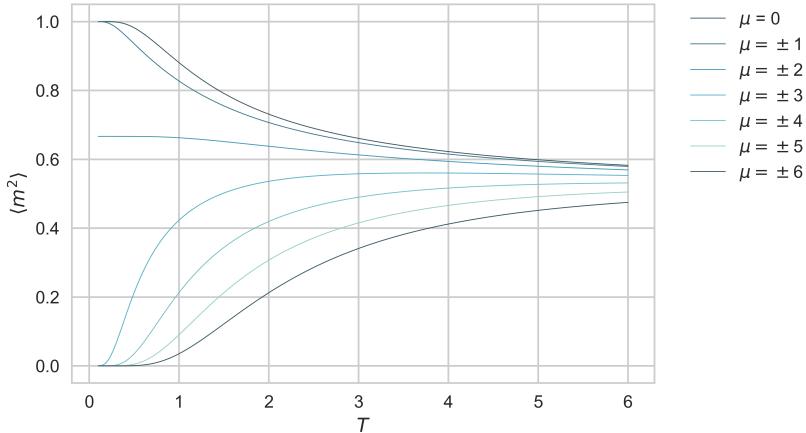


Figure 2.6: Magnetization as a function of temperature $\langle m^2 \rangle (T)$ in the single site Hubbard model for varying chemical potential μ . Local moments develop at lower temperature. However, as we increase the magnitude of the chemical potential, the situation is reversed. At low temperatures, the site is either doubly occupied or empty, and so the magnetization goes to zero. Thermal fluctuations allow the occupation of the site to fluctuate, and the magnetization to become nonzero.

2.3.2 The non-interacting ($\frac{U}{t} = 0$) limit

In the $\frac{U}{t} = 0$ limit, the spin sectors become independent (since the opposite spin electrons do not interact via the on-site term) and they may be considered separately. Thus, we omit the spin indexes

of the operators in the Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) - \mu \sum_i n_i = \mathbf{c}^\dagger \left(-t\mathbf{K} - \mu\mathbf{I} \right) \mathbf{c}, \quad (2.40)$$

where we casted the Hamiltonian as a bilinear form, and defined

$$\mathbf{c} = \begin{bmatrix} c_1 & c_2 & \dots & c_N \end{bmatrix}^T \quad \mathbf{c}^\dagger = \begin{bmatrix} c_1^\dagger & c_2^\dagger & \dots & c_N^\dagger \end{bmatrix}, \quad (2.41)$$

and where \mathbf{I} is the identity matrix. We also defined a matrix of zeros and ones specifying the hopping geometry, \mathbf{K} . The elements of the hopping matrix are simply defined by the indicator function: $K_{ij} = \mathbb{1}_{\langle j_i \rangle}(i)$, where $\langle j_i \rangle$ is the set of neighbors j of site i . When writing down \mathbf{K} , we must specify the boundary conditions. Periodic boundary conditions (PBCs) preserve a system's translational invariance and are advantageous because they reduce finite size effects. An example of a quantity which is measured more accurately is energy. In the thermodynamic limit, $N \rightarrow \infty$, the measured energy differs from the actual value by a correction of order $\mathcal{O}(\frac{1}{N^2})$ with PBCs, while for Open boundary conditions (OBCs), the correction is of order $\mathcal{O}(\frac{1}{N})$ [56]. Additionally, PBCs have the property of giving site independent observables. For example, the electron density per site does not vary with the distance to the edges of the lattice with PBCs, but it does when we use OBCs.

For concreteness, let us consider a rectangular two-dimensional lattice with $N_x \times N_y$ sites. Then, we have $\dim(\mathbf{K}) = N_x N_y \times N_x N_y$, and

$$\mathbf{K} = \mathbf{I}_y \otimes \mathbf{K}_x + \mathbf{I}_x \otimes \mathbf{K}_y, \quad (2.42)$$

where $\mathbf{I}_{x,y}$ are identity matrices of dimension $N_{x,y} \times N_{x,y}$, respectively, and $\mathbf{K}_{x,y}$ are the hopping matrices in the x and y -directions. For lattices in 1D or 2D, it is possible to find an exact eigendecomposition

$$\mathbf{K} = \mathbf{F}^T \boldsymbol{\Lambda} \mathbf{F} \quad \text{with} \quad \mathbf{F}^T \mathbf{F} = \mathbf{I}, \quad (2.43)$$

where $\boldsymbol{\Lambda} = \text{diag}(\lambda_{\mathbf{k}})$ is a diagonal matrix of eigenvalues of \mathbf{K} . The Hamiltonian is diagonalized:

$$\mathcal{H} = \tilde{\mathbf{c}}^\dagger \left(-t\mathbf{K} - \mu\mathbf{I} \right) \tilde{\mathbf{c}} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \tilde{n}_{\mathbf{k}}, \quad (2.44)$$

where $\tilde{\mathbf{c}} = \mathbf{F}\mathbf{c}$ and $\tilde{\mathbf{c}}^\dagger = (\mathbf{F}\mathbf{c})^\dagger$, and

$$\varepsilon_{\mathbf{k}} = -t\lambda_{\mathbf{k}} - \mu \quad \tilde{n}_{\mathbf{k}} = \tilde{c}_{\mathbf{k}}^\dagger \tilde{c}_{\mathbf{k}} \quad (2.45)$$

This is equivalent to performing a canonical transformation on the annihilation (creation) operators, that preserves not their Poisson brackets, as in classical mechanics, but their anti-commutators. Finding the eigendecomposition is equivalent to changing to Fourier space:

$$\tilde{c}_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum e^{i\mathbf{k} \cdot \mathbf{R}_j} c_j^\dagger, \quad (2.46)$$

a transformation which indeed preserves the anti-commutation relations, and the total number operator, i.e., $n = \sum_j n_j = \tilde{n} = \sum_{\mathbf{k}} n_{\mathbf{k}}$. The $\tilde{c}_{\mathbf{k}}$ -operators are equally valid electron creation/annihilation operators, obeying the same anticommutation relations as the original operators c_i , and the total number operator is unchanged under our transformation. However, while the original operators create/annihilate particles at specific (spatial) sites, the new ones create/annihilate particles with momentum \mathbf{k} . Both sets of operators describe the same physics. Why can't this procedure be applied to the interacting case? Well, for instance, the interaction term in the Hubbard model takes on a fairly complex form in momentum space so it is not possible to apply a similar transformation to diagonalize it.

Now, it turns out that it is easy to evaluate the partition function for quadratic Hamiltonians. If $\mathcal{H} = \mathbf{c}^\dagger \mathbf{H} \mathbf{c}$, where \mathbf{H} is a $N \times N$ Hermitian matrix, then we have that

$$\text{Tr}[e^{-\beta \mathcal{H}}] = \prod_{i=1}^N (1 + e^{-\beta \lambda_i}), \quad (2.47)$$

where λ_i are the eigenvalues of \mathbf{H} . We present a proof of this result in appendix A. It suggests that if we are able to devise some approximation to transform the quartic term of the interacting Hubbard model in a quadratic form, then we can solve it. While this idea is essentially correct, the procedure is not straightforward. Actually, we explore this in the next chapter to derive the simulation method that is at the basis of this work.

To complete the solution of the non-interacting case we apply the result of equation (2.47) to compute the partition function corresponding to the quadratic Hamiltonian defined in equation (2.44):

$$Z = \prod_{\mathbf{k}} (1 + e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)}), \quad (2.48)$$

where $\varepsilon_{\mathbf{k}}$ is just the dispersion relation for a tight binding model, a standard result. A related quantity is the density of states, counting the number of states with a given energy. For a single spin species:

$$N(E) = \frac{1}{N} \sum_{\mathbf{k}} \delta_{E, \varepsilon_{\mathbf{k}}} \rightarrow \frac{1}{(2\pi)^d} \int d\mathbf{k} \delta(E - \varepsilon_{\mathbf{k}}) \text{ when } N \rightarrow \infty. \quad (2.49)$$

In 1D, we have $\varepsilon_k = -2t \cos k$, which gives $N(E) = (\pi\sqrt{4t^2 - E^2})^{-1}$ (see appendix A).

Now that we have found a closed form solution for Z , it is again possible to find closed form expressions for observables of interest as well, namely:

1. the density, or average occupation of each site, ρ .

$$\rho = \langle n \rangle = \langle \tilde{n} \rangle = \frac{1}{N} \sum_{\mathbf{k}} \langle \tilde{n}_{\mathbf{k}} \rangle = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{1 + e^{\beta(\varepsilon_{\mathbf{k}} - \mu)}} = \frac{1}{N} \sum_{\mathbf{k}} f_{\mathbf{k}}, \quad (2.50)$$

where $f_{\mathbf{k}} = (1 + e^{\beta(\varepsilon_{\mathbf{k}} - \mu)})^{-1}$ is the Fermi-Dirac distribution (at half filling: $\mu = 0$).

2. the energy $E = \langle \mathcal{H} \rangle$.

$$E = \frac{1}{N} \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}} - \mu}{1 + e^{\beta(\varepsilon_{\mathbf{k}} - \mu)}} = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) f_{\mathbf{k}} \quad (2.51)$$

3. the equal-time Green's function, which plays a key role in computing other quantities, such as correlation functions.

$$G_{l,j} = \langle c_l c_j^\dagger \rangle = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{l}-\mathbf{j})} (1 - f_{\mathbf{k}}) \quad (2.52)$$

Note that the Green's function, like the Hamiltonian, is translationally invariant: $G_{l,j} = G_{l-j}$. If we use PBCs, no site is singled out, they are all equivalent and this behavior of the Green's function should become apparent in our simulations.

The properties of a fermionic system are dominated by particles near the Fermi surface. On the square lattice, a unique feature called perfect nesting appears. For example, in 2D, the wavevector $\mathbf{k} = (\pi, \pi)$ connects symmetric regions of the Fermi surface. This suggests that this wavevector could have a crucial role in the description of the model in the square lattice. Indeed, as we will see, a large magnetic structure factor at $\mathbf{k} = (\pi, \pi)$ signals antiferromagnetic order. This is a feature of the Hubbard model at half filling down to $U = 0$. A similar effect happens in 1D, at $k = \pi$.

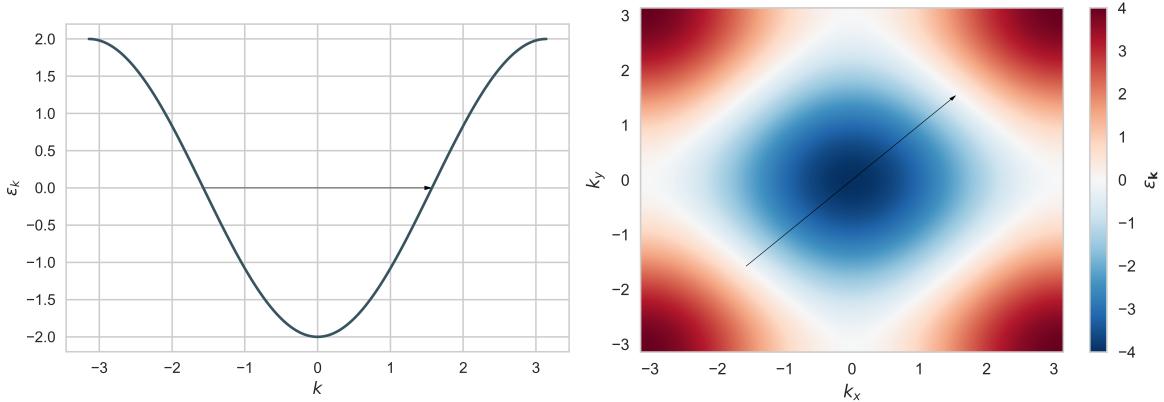


Figure 2.7: Dispersion relations for the 1D chain and the square lattice in the non-interacting case. For the square lattice, the surfaces separating the different colors are Fermi surfaces for different fillings of the lattice. In particular, for half filling ($\rho = 1, \mu = 0$), we obtain the rotated square in the white region.

From our analysis, we draw an important conclusion: that solving the single-particle problem, that is, obtaining $\varepsilon_{\mathbf{k}}$, gives us all the information we need about all particle sectors (any number of particles, which is controlled via the chemical potential). When the on-site interaction is “turned off”, the fermions simply occupy the one-particle states according to Pauli’s exclusion principle. The single-particle sector allows us to extrapolate to obtain the behavior of a system for any number of particles simply because $U = 0$; even if the hoppings were not uniform, this would hold. The hoppings need not even be only between nearest neighbors, and in general we could even consider a chemical potential varying from site to site. All we require is that the Hamiltonian is a quadratic form of the fermion operators.

2.4 Exact Diagonalization and the Heisenberg Hamiltonian as the Effective $\frac{U}{t} \gg 1$ Model

In appendix A, we argue that Mott insulators allow low energy magnetic excitations (spin flips) without incurring into any energy cost whatsoever. Their insulating phase corresponds to a configuration where each atom has an odd number of electrons, let's say one. This electron may have its spin up or down. In the purely atomic limit $\frac{U}{t} \rightarrow \infty$, the atoms are infinitely far, and the excitation spectrum is very simple. The ground state is highly degenerate: every configuration with one electron per site is a ground state. As a matter of fact, the ground state is 2^N -fold degenerate. The first excited state corresponds to configurations with a hole and a doubly occupied site. Let us set the energy of the ground state to zero in our conventions. The energy of these configurations is then U , and there are $N(N - 1)2^{N-2}$ of them. This process of generating higher energy excitations may be continued.

When the atoms are brought together, the first effect is the lifting of the degeneracy of the ground state, i.e. the splitting of the subspace of energy $E = 0$. The effective Hamiltonian describing the lifting of the degeneracy of the lowest energy band is obtained by applying degenerate perturbation theory [79] to the kinetic term of the Hubbard Hamiltonian⁶

$$\mathcal{H}_0 = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \quad (2.53)$$

2.4.1 Two-site calculation

The effect of the hopping term is best understood in a minimal two-site example. There are four one-particle quantum states, represented by the action of the operators $c_{1,\uparrow}^\dagger, c_{1,\downarrow}^\dagger, c_{2,\uparrow}^\dagger, c_{2,\downarrow}^\dagger$ on the vacuum state. There are six two-particle states in the Fock space represented by $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle$:

$$\begin{aligned} |1\rangle &\equiv |1, 0, 1, 0\rangle = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger |0\rangle & |2\rangle &\equiv |0, 1, 0, 1\rangle = c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger |0\rangle \\ |3\rangle &\equiv |1, 0, 0, 1\rangle = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle & |4\rangle &\equiv |0, 1, 1, 0\rangle = c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle \\ |5\rangle &\equiv |1, 1, 0, 0\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle & |6\rangle &\equiv |0, 0, 1, 1\rangle = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle \end{aligned} \quad (2.54)$$

The two-site Hamiltonian

$$\mathcal{H}_2 = -t \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\uparrow}^\dagger c_{1\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) + U \left(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow} \right) \quad (2.55)$$

acts on the states of the Fock space as follows

⁶An alternative method would be to use a canonical transformation technique.

$$\begin{aligned}
\mathcal{H}_2 |1\rangle &= 0 \\
\mathcal{H}_2 |2\rangle &= 0 \\
\mathcal{H}_2 |3\rangle &= -t(c_{2\uparrow}^\dagger c_{1\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow})c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle = -t(|5\rangle + |6\rangle) \\
\mathcal{H}_2 |4\rangle &= -t(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow})c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |0\rangle = t(|5\rangle + |6\rangle) \\
\mathcal{H}_2 |5\rangle &= \left[-t(c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow}) + Un_{1\uparrow}n_{1\downarrow} \right] c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle = U|5\rangle - t(|3\rangle - |4\rangle) \\
\mathcal{H}_2 |6\rangle &= \left[-t(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow}) + Un_{2\uparrow}n_{2\downarrow} \right] c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle = U|6\rangle - t(|3\rangle - |4\rangle)
\end{aligned} \tag{2.56}$$

When we act on the first two states we obtain 0 because every term of the Hamiltonian gives a term $(c^\dagger)^2$, which is 0 due to Pauli's exclusion principle. The minus signs that appear on the hopping terms stem from the fermion anticommutation relations.

Let us now diagonalize the Hamiltonian in the subspace spanned by $\{|3\rangle, |4\rangle, |5\rangle, |6\rangle\}$. If we add states $|3\rangle$ and $|4\rangle$, we get 0 when acting with the Hamiltonian.

$$\mathcal{H}_2(|3\rangle + |4\rangle) = 0 \tag{2.57}$$

On the other hand, if we subtract $|5\rangle$ and $|6\rangle$, we obtain

$$\mathcal{H}_2(|5\rangle - |6\rangle) = U(|5\rangle - |6\rangle) \tag{2.58}$$

We have found two more eigenvalues (the first two were trivially found to be zero). The others are found by subtracting $|3\rangle$ and $|4\rangle$ and adding $|5\rangle$ and $|6\rangle$.

$$\begin{aligned}
\mathcal{H}_2(|3\rangle + |4\rangle) &= -2t(|5\rangle + |6\rangle) \\
\mathcal{H}_2(|5\rangle - |6\rangle) &= -2t(|3\rangle - |4\rangle) + U(|5\rangle + |6\rangle)
\end{aligned} \tag{2.59}$$

The characteristic equation allowing us to find the rest of the eigenvalues in the rotated subspace spanned by $\{|3\rangle \pm |4\rangle, |5\rangle \pm |6\rangle\}$ is

$$E(E - U) - 4t^2 = 0 \iff E_\pm = \frac{U \pm \sqrt{U^2 + 16t^2}}{2} \tag{2.60}$$

Taylor expanding the square root up to second order, we obtain

$$E_- = -\frac{4t^2}{U} \quad E_+ = U + \frac{4t^2}{U} \tag{2.61}$$

Thus, we have obtained the complete energy spectrum. The ground state is a non-degenerate state of energy $-\frac{4t^2}{U}$, while the first excited state is a 3-fold degenerate state with energy 0. The two other excited states have energies of the order of U , the first one being exactly U and the second $U + \frac{4t^2}{U}$.

There are four states for which the energy would be 0 if the hopping term vanished, corresponding to the four states with one electron per site. The effect of the hopping term is to lift the degeneracy by

splitting the 4-fold degenerate zero energy state into a singlet of energy $-\frac{4t^2}{U}$ and a triplet of energy 0. This is what we obtain by minimizing a Heisenberg Hamiltonian of the form

$$\mathcal{H} = \frac{4t^2}{U} \left(\mathbf{S}_1 \cdot \mathbf{S}_2 - \frac{1}{4} \right) \quad (2.62)$$

for two spins- $\frac{1}{2}$. However, it turns out that this result is yet more general. For an arbitrary number of sites, this is the form of the effective Hamiltonian at second order (see appendix (A) for details).

It is easy to extend this analysis beyond half filling to compare it to our solution for the single site case. The latter gave us some insight into how the on-site interaction gives rise to magnetic ordering, and about the development of the Mott plateau. Adding in the hopping we can understand the interplay between kinetic and potential energy, and the magnetic correlations between sites. In fact, we will outline the simplest nontrivial method to solve Hubbard-type Hamiltonians: *exact diagonalization*, which is a competitor of QMC, but is limited to very small system sizes.

Since the two-site Hamiltonian of equation (2.55) commutes with n_σ , it conserves the number of up and down fermions, and the $2^4 = 16$ states can be divided into 9 sectors of varying dimension d : $(n_\uparrow, n_\downarrow, d) = (0, 0, 1), (1, 0, 2), (2, 0, 1), (0, 1, 2), (1, 1, 4), (2, 1, 2), (0, 2, 1), (1, 2, 2), (2, 2, 1)$. There are four sectors of dimension 1: the empty lattice, the fully filled lattice, and the lattices with two-like spin fermions. All these sectors have zero kinetic energy: in the first, there are no electrons present to hop, and in the second Pauli's exclusion principle blocks hopping. The sectors with $n_\sigma = 2$ have energy $-U/2$, while the ones with $n_\uparrow = n_\downarrow$ have energy $U/2$.

The four sectors of dimension 2 are also simple. One and three particle sectors must have the same energy spectrum due to Particle-hole symmetry (PHS). They have eigenenergies $\pm t$. A single fermion can hop between sites, while out of the three fermions, the two with like-spin are blocked and can't hop to the same site, leaving a single fermion free to hop. We have already solved the most complicated $n_\uparrow = n_\downarrow = 1$ sector, while tackling the half filled case. By determining the complete spectrum of the two-site Hubbard model, we demonstrated that the eigenenergies in the $U \neq 0$ case can't be deduced solely from considering the single-particle sector. The low temperature properties of the model are determined by the lowest energy eigenvalues, which all seem to fall in the half filled sectors. Subtracting $U/2$ to the energies we obtained in the half filled sectors is equivalent to considering the PHS form of the Hamiltonian. At half filling, we end up with four states with energies around $-U/2$ (the so called lower Hubbard band), and two states with energies around $U/2$ (the so called upper Hubbard band). The lower Hubbard band controls the low temperature physics. In the next section, we show that the Heisenberg Hamiltonian that seems to govern the behavior of the electrons in the lower Hubbard band is in fact the effective $U/t \gg 1$ Hamiltonian.

2.4.2 Degenerate perturbation theory

To first order in \mathcal{H} , the matrix elements of its effective Hamiltonian coincide in the ground state subspace, by definition.

$$\langle m | \mathcal{H}_{\text{eff}} | n \rangle = \langle m | \mathcal{H}_0 | n \rangle , \quad (2.63)$$

where $|m\rangle$, and $|n\rangle$ belong to the ground state subspace. Since we are considering the system to be at half filling in our calculations, $|m\rangle$, and $|n\rangle$ must have one electron per site. The hopping Hamiltonian \mathcal{H}_0 makes an electron hop, leaving its previous site empty, and the site it hops to doubly occupied. This implies that all the matrix elements in the previous equation must be 0.

To second order, the matrix elements of the effective Hamiltonian are

$$\langle m|\mathcal{H}_{\text{eff}}|n\rangle = \sum_{|k\rangle} \frac{\langle m|\mathcal{H}_0|k\rangle \langle k|\mathcal{H}_0|n\rangle}{E_0 - E_k} = -\frac{1}{U} \sum_{|k\rangle} \langle m|\mathcal{H}_0|k\rangle \langle k|\mathcal{H}_0|n\rangle, \quad (2.64)$$

where $|k\rangle$ are the states that are not in the ground state subspace. In the second equality we simply noted that \mathcal{H}_0 creates a doubly occupied site. The energy cost of creating a doubly occupied site is U .

The identity operator in the in the subspace of states with one doubly occupied site $\sum_{|k\rangle} |k\rangle\langle k|$ may be written in a more convenient form in another representation: $\sum_j n_{j,\sigma} n_{j,-\sigma}$, so that the effective Hamiltonian becomes

$$\mathcal{H}_{\text{eff}} = -\mathcal{H}_0 \frac{\sum_j n_{j,\sigma} n_{j,-\sigma}}{U} \mathcal{H}_0 \quad (2.65)$$

In appendix (A), we find the Heisenberg model as the effective Hamiltonian in this $\frac{U}{t} \gg 1$ limit. This is consistent since the Heisenberg model couples spins on different sites, thus it is an *atomic* model.

$$\mathcal{H}_{\text{eff}} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (2.66)$$

with $J = 4t^2/U$. Since $J > 0$, the model favors configurations with antiparallel adjacent spins.

There is an intuitive physical picture for this result: if two electrons on neighboring sites have parallel spins, none of the two can hop to the neighboring site due to Pauli's exclusion principle. If adjacent sites have antiparallel spins, however, it is possible for any of the two electrons to hop to the neighboring site, and an exchange process allows the system to lower its energy. First, a fermion hops to a neighboring site already occupied with an opposite spin fermion. The intermediate state has a higher energy by U . Then, the fermion hops back to its original site, in a process that decreases the energy: $E^{(2)} \propto -t^2/U$. We found the correct factor, giving the coupling constant $J = 4t^2/U$.

2.5 Green's functions and Wick's theorem

Green's functions are the core of the first perturbative, diagrammatic approaches to the Hubbard model. They are very useful in reducing the enormous amount of variables that come into play in correlated systems to a manageable number. Here we try do give some intuition about how they work since they are the central quantity in the QMC method we will use. For a very complete and thorough description of the ideas in this section see [80].

Considering the imaginary-time variable of the previous chapter $\tau = it$, for $\tau > 0$, the Green's function is defined as

$$G_{ij}(\tau, 0) = \langle c_i(\tau) c_j^\dagger(0) \rangle, \text{ with } c_i(\tau) = e^{\mathcal{H}\tau} c_i(0) e^{-\mathcal{H}\tau} \quad (2.67)$$

2.5.1 Single site case

The Hubbard Hamiltonian does not distinguish between spin-up and spin-down sectors. Thus, without loss of generality, let us consider the spin-up sector, and compute $G_\uparrow(\tau, 0) = \langle c_\uparrow(\tau) c_\uparrow^\dagger(0) \rangle$. Only the states $|n_\uparrow n_\downarrow\rangle = |00\rangle, |01\rangle$ contribute to the expectation due to the creation operator on the right, which gives 0, unless there is no spin up electron already in the state it acts upon.

$$\begin{aligned} c_\uparrow(\tau) c_\uparrow^\dagger(0) |00\rangle &= e^{\mathcal{H}\tau} c_\uparrow(0) e^{-\mathcal{H}\tau} c_\uparrow^\dagger(0) |00\rangle = e^{\mathcal{H}\tau} c_\uparrow(0) e^{-\mathcal{H}\tau} |01\rangle \\ &= e^{\mathcal{H}\tau} c_\uparrow(0) e^{U\tau/4+\mu\tau} |10\rangle = e^{\mathcal{H}\tau} e^{U\tau/4+\mu\tau} |00\rangle = e^{U\tau/2+\mu\tau} |00\rangle \\ c_\uparrow(\tau) c_\uparrow^\dagger(0) |01\rangle &= e^{\mathcal{H}\tau} c_\uparrow(0) e^{-\mathcal{H}\tau} c_\uparrow^\dagger(0) |01\rangle = e^{\mathcal{H}\tau} c_\uparrow(0) e^{-\mathcal{H}\tau} |11\rangle \\ &= e^{\mathcal{H}\tau} c_\uparrow(0) e^{-U\tau/4+2\mu\tau} |11\rangle = e^{\mathcal{H}\tau} e^{-U\tau/4+2\mu\tau} |01\rangle = e^{U\tau/2+\mu\tau} |01\rangle \end{aligned} \quad (2.68)$$

Using the expression for the partition function that we obtained in equation (2.31), we arrive at

$$G_\uparrow(\tau, 0) = \frac{e^{\tau(U/2+\mu)} e^{-\beta U/4} + e^{-\tau(U/2-\mu)} e^{\beta(U/4+\mu)}}{e^{-\beta U/4}(1 + 2e^{\beta(U/2+\mu)} + e^{2\beta\mu})}, \quad (2.69)$$

which, at half filling becomes

$$G_\uparrow(\tau, 0) = \frac{e^{\tau U/2} e^{-\beta U/4} + e^{-\tau U/2} e^{\beta U/4}}{2e^{-\beta U/4} + 2e^{\beta U/4}}, \quad (2.70)$$

There is a well known relation between the Green's function and the spectral density $A(\omega)$, which may be regarded as a local density of states:

$$G(\tau, 0) = \int_{-\infty}^{+\infty} A(\omega) \frac{e^{-\omega\tau}}{e^{-\beta\omega} + 1} d\omega, \quad (2.71)$$

If we replace the following expression for the spectral density in equation (2.71), we recover the result for the half filled case.

$$A(\omega) = \frac{1}{2} \left(\delta(\omega - \frac{U}{2}) + \delta(\omega + \frac{U}{2}) \right) \quad (2.72)$$

We could do a similar calculation for $\mu \neq 0$ by changing the spectral density adequately, but the algebra is slightly more cumbersome, and the result does not bring additional insight.

The spectral density consists of two delta functions separated by U , which is reminiscent of our result for the Mott insulating gap. In the same way that the gap softens (eventually disappearing) when we introduce hopping, the spectral function for the full Hubbard Hamiltonian changes accordingly, reflecting the same information about the properties of the system as the Green's function, encoded in a different manner. In QMC, we can access $G(\tau, 0)$ and deduce the properties of the system from it.

2.5.2 Non-interacting case

In this limit, we can compute $G_{ij}(\tau, 0)$ analytically by going to momentum space.

$$c_{\mathbf{k}}(\tau) = e^{\mathcal{H}\tau} c_{\mathbf{k}}(0) e^{-\mathcal{H}\tau} = e^{-\varepsilon_{\mathbf{k}}\tau} c_{\mathbf{k}}(0) \quad (2.73)$$

This equation can be verified by acting with the left hand side and with right hand side on the states $|0\rangle$ and $|1\rangle$, and noting that the result is the same. Alternatively, one can use the equation of motion $\partial_{\tau}\hat{A}(\tau) = [\mathcal{H}, \hat{A}(\tau)]$. To generalize the result of equation (2.52) for the *equal-time* Green's function to *unequal-time* we transform the fermionic operators in G to momentum space, and use $\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \rangle = 1 - f_{\mathbf{k}}$ to obtain

$$G_{ij}(\tau, 0) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} (1 - f_{\mathbf{k}}) e^{-\varepsilon_{\mathbf{k}}\tau}, \quad (2.74)$$

which is translationally invariant corresponding to the symmetry of the Hamiltonian.

We can generalize our definition of the Green's function by using the time-ordering operator \mathcal{T} :

$$G_{\mathbf{k}}(\tau, 0) = -\langle \mathcal{T} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger(0) \rangle, \quad (2.75)$$

where

$$\mathcal{T} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger(0) = \begin{cases} c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger(0), & \tau > 0 \\ -c_{\mathbf{k}}^\dagger(0) c_{\mathbf{k}}(\tau), & \tau < 0 \end{cases} \quad (2.76)$$

An important property follows immediately from this definition: $G(\tau + \beta, 0) = -G(\tau, 0)$ for $-\beta < \tau < 0$. The imaginary-time anti-periodicity constraint implies that the frequencies that appear when we Fourier transform are the so called (fermionic) Matsubara frequencies $\omega_n = \frac{(2n+1)\pi}{\beta}$.⁷

$$G(i\omega_n) = \int_0^{\beta} \frac{d\tau}{\beta} G(\tau, 0) e^{i\omega_n \tau} \quad G(\tau) = \sum_n G(i\omega_n) e^{-i\omega_n \tau} \quad (2.77)$$

In momentum space, and imaginary time, the Green's function then become

$$G_{\mathbf{k}}(\tau, 0) = \begin{cases} -e^{-\varepsilon_{\mathbf{k}}} (1 - f_{\mathbf{k}}), & 0 < \tau < \beta \\ e^{-\varepsilon_{\mathbf{k}}} f_{\mathbf{k}}, & -\beta < \tau < 0, \end{cases} \quad (2.78)$$

which leads to

$$G_{\mathbf{k}}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}}} \quad (2.79)$$

in frequency space. This result may also be obtained by taking the partial derivative of the time-ordered Green's function written in the form $G_{\mathbf{k}}(\tau, 0) = \langle c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger(0) \rangle \theta(\tau) - \langle c_{\mathbf{k}}(0) c_{\mathbf{k}}^\dagger(\tau) \rangle \theta(-\tau)$ and Fourier transforming both sides to solve for $G(i\omega_n)$. Taking a time derivative of G implies computing commutators of \mathcal{H} with the fermionic operators. The equation closes for quadratic Hamiltonians, which

⁷Analogously, for bosons, imaginary-time periodicity implies that $\omega_n = 2n\pi/\beta$

we, of course, know to be soluble.

2.5.3 Finite temperature Wick's theorem for fermions

As was emphasized in section 2.3, the key concept that will be used in deriving the auxiliary field method is a mapping to a single-particle problem defined in terms of a quadratic Hamiltonian. Thus, Wick's theorem may be applied to simplify products of fermionic operators. In [80], the theorem is rigorously proven for both the ground state and the finite temperature cases. Here, we summarize the elements that will be useful in the next chapter, and leave a more detailed discussion following the discussion of [81] to appendix A.

In general, Green's functions are a much more complicated object than in the simple examples treated so far. Fortunately, our mapping to a single particle problem allows us to express many-particle Green's functions as a function of single particle Green's functions sampled over the auxiliary field's configurations. The latter will turn out to play a crucial role in the sampling process itself. Moreover, any observable may be written in terms of these single particle Green's functions (for a given auxiliary field configuration) by using Wick's theorem. Thus, measuring any observable requires simply gathering the necessary elements of the single particle Green's function, since the latter must be computed already to sample the auxiliary field's configurations. This observation stems solely from the fact that the electrons are decoupled once the auxiliary field is introduced, reducing the interacting problem to a single particle problem.

The single particle (equal-time) Green's function for a fixed field configuration \mathbf{h} is defined as $G_{ij} \equiv \langle c_i c_j^\dagger \rangle_{\mathbf{h}}$. Any observable of interest is reduced to a sum of terms of type

$$\begin{aligned} \langle c_{i_1}^\dagger c_{i_2} c_{i_3}^\dagger c_{i_4} \rangle_{\mathbf{h}} &= \langle c_{i_1}^\dagger c_{i_2} \rangle_{\mathbf{h}} \langle c_{i_3}^\dagger c_{i_4} \rangle_{\mathbf{h}} + \langle c_{i_1}^\dagger c_{i_4} \rangle_{\mathbf{h}} \langle c_{i_2} c_{i_3}^\dagger \rangle_{\mathbf{h}} \\ &= (\delta_{i_1 i_2} - G_{i_2 i_1}) (\delta_{i_3 i_4} - G_{i_4 i_3}) + (\delta_{i_1 i_4} - G_{i_4 i_1}) G_{i_2 i_3}, \end{aligned} \quad (2.80)$$

by using Wick's theorem, and the fact that the Hamiltonian conserves the particle number. As we shall see later, an analogous relation holds for quantities defined of *time-displaced* Green's functions. The proof consists of writing those quantities in terms of a combination of equal-time Green's functions and matrices that represent the single particle propagators. After this step, one can write a version of Wick's theorem for time-displaced Green's functions.

2.6 Magnetism and mean field theory

In this section we will build a picture of magnetism in the Hubbard model in increasing level of sophistication. As our degenerate perturbation theory calculation of section (2.4) showed, the on-site interaction favors the situation in which neighboring fermions have opposite spins through an Heisenberg type interaction. A different approach leads to the Stoner criterion for ferromagnetism. The argument is based on creating an imbalance between the numbers of spin-up and spin-down fermions, and analyzing the interplay between the resulting increase in kinetic energy, and decrease

in potential energy. Finally, we formulate a (static) mean field theory for the Hubbard model, and discuss how it relates to the non-interacting case.

2.6.1 Stoner criterion for ferromagnetism

Pauli's exclusion principle gives a prescription on how to fill fermionic energy levels so as to yield the lowest possible total energy. Start from the lowest level, and start filling each level of higher energy consecutively with two electrons, one of each spin. This procedure requires the number of spin-up and spin-down electrons to be the same. Otherwise, there is an energy cost, since we are obliged to fill higher energy levels with the excess electrons.

An unequal number of spin-up and spin-down electrons also decreases the potential energy. An extreme example is a completely polarized lattice. In that case, the potential energy is zero. More generally, partial spin polarization makes double occupation unlikely, lowering the potential energy.

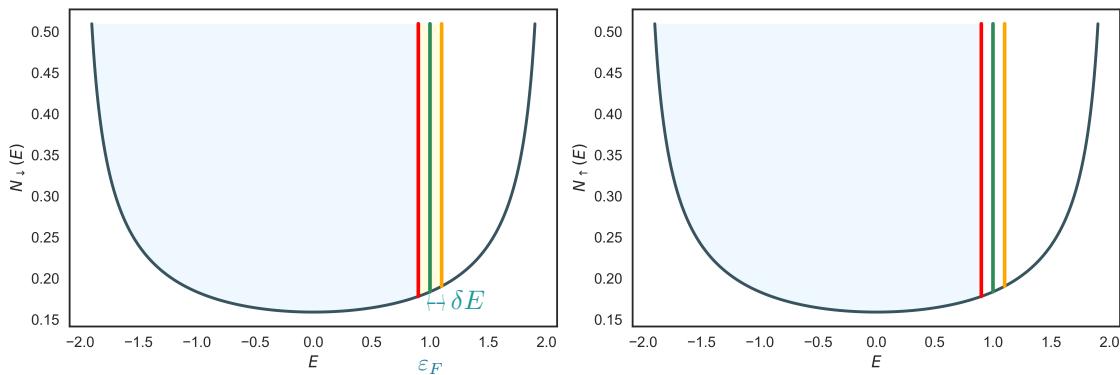


Figure 2.8: Density of states of the 1D tight-binding model. Here we represent a polarization of the spins, which leads to an increase in kinetic energy, since the imbalance of spins forces higher energy levels to be filled.

A system with density of states $N(E)$ has equal densities of spin-up and spin-down electrons, n , filling the energy levels up to the Fermi energy, ε_F . When we reduce, say the spin-up electron density by δn , the potential energy is lowered by $\delta P = U(n + \delta n)(n - \delta n) - Un^2 = -U(\delta n)^2$.

The extra density of electrons δn that is added to the down sector will occupy levels with energy greater than ε_F , so that $\delta n = N(\varepsilon_F)\delta E$. Some spin-up levels below ε_F that used to be occupied are now empty, which makes δn fermions per site increase their energy by δE , leading to a change in kinetic energy $\delta K = \delta n\delta E = \frac{(\delta n)^2}{N(\varepsilon_F)}$. The global change in energy is

$$\delta E = \delta P + \delta K = \left(-U + \frac{1}{N(\varepsilon_F)} \right) (\delta n)^2 = \left(-UN(\varepsilon_F) + 1 \right) \frac{(\delta n)^2}{N(\varepsilon_F)} \quad (2.81)$$

If $UN(\varepsilon_F) > 1$, then $\delta E < 0$, and the imbalance of spin densities actually becomes more favorable. Thus, magnetism is favored by a large on-site interaction and a large density of states at (near) the Fermi energy.

2.6.2 Mean field theory of the Hubbard model

We have already encountered an example of a mean field theory when deriving the Hubbard Hamiltonian (see appendix A, where we provide motivation both heuristically and via a more rigorous variational approach). In mean field theory, we give a systematic procedure to derive the most plausible quadratic Hamiltonian (which, as we know by now, is soluble) capturing some of the physics of our system. In the case of the Hubbard model, to find the best possible approximation for the quartic term we start by expressing the number operators in terms of an average plus fluctuations: $n = \langle n \rangle + (n - \langle n \rangle) \equiv \langle n \rangle + \delta n$. Then, we make this substitution in the interaction term and neglect the term that is second order in the fluctuations to obtain

$$\begin{aligned} n_\uparrow n_\downarrow &= \left[\langle n_\uparrow \rangle + (n_\uparrow - \langle n_\uparrow \rangle) \right] \left[\langle n_\downarrow \rangle + (n_\downarrow - \langle n_\downarrow \rangle) \right] \\ &= \langle n_\uparrow \rangle \langle n_\downarrow \rangle + \langle n_\downarrow \rangle (n_\uparrow - \langle n_\uparrow \rangle) + \langle n_\uparrow \rangle (n_\downarrow - \langle n_\downarrow \rangle) + \mathcal{O}((\delta n)^2) \\ &= n_\uparrow \langle n_\downarrow \rangle + n_\downarrow \langle n_\uparrow \rangle - \langle n_\uparrow \rangle \langle n_\downarrow \rangle \end{aligned} \quad (2.82)$$

We consider a “mean field” in the sense that the average density of spin-up electrons interacts with the spin-down electrons and vice-versa. The last term subtracts the overcounted original single interaction term. From equation (2.82), we obtain the quadratic mean field Hamiltonian

$$\mathcal{H}_{\text{MF}} = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i \left(n_{i,\uparrow} \langle n_{i,\downarrow} \rangle + n_{i,\downarrow} \langle n_{i,\uparrow} \rangle - \langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle \right) \quad (2.83)$$

To solve \mathcal{H}_{MF} , one merely has to diagonalize the corresponding matrix. In the ferromagnetic case, the average occupation is independent of the specific site, but can vary with the spin species: $n_{i,\uparrow(\downarrow)} = n \pm m$, where m is the magnetization, the order parameter of the transition to a ferromagnetic phase. Similarly, for the AF case on a bipartite lattice, we consider $n_{i,\uparrow(\downarrow)} = n \pm (-1)^i m$, leading to a staggered potential.

Now we take on a Landau Ginzburg theory kind of approach. We compute the energy E for fixed n as a function of m , and inspect the system for ferromagnetic ordering: if the minimum lies at $m = 0$, the system is paramagnetic, otherwise it is ferromagnetic. For simplicity, let us now consider the 1D model. Since the average densities are site-independent, we can easily write down the polarized dispersion relations (up to an additive constant):

$$\varepsilon_{\uparrow k} = U(n - m) - 2t \cos k \quad \varepsilon_{\downarrow k} = U(n + m) - 2t \cos k, \quad (2.84)$$

and add these levels up for the various possible fillings of the lattice.

The computational procedure to perform mean field computations goes as follows:

- Fix the lattice size N , the total particle number N_p , and the on-site interaction U .
- Set the possible densities by iterating $N_\uparrow = 0, 1, \dots, N_p/2$, and $N_\downarrow = N_p - N_\uparrow$ (we only need half the values since the values are symmetric under $N_\uparrow \leftrightarrow N_\downarrow$), and setting $n_{\uparrow,\downarrow} = N_{\uparrow,\downarrow}/N$.

- Fill the lowest N_{\uparrow} , and N_{\downarrow} energy levels, by looping over the allowed momentum states $k = \frac{2\pi}{N} \{-\frac{N}{2} + 1, -\frac{N}{2}, \dots, \frac{N}{2}\}$, and using equation (2.84). Normalize the energy to N and add in the additive constant $-\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle$. This step is altered for the AF case since we are assuming the up and down densities to be identical over the whole lattice. In such case, we fix $n = N_p/2$ and loop over $m = 1/N, 2/N, \dots$, staying within the first Brillouin zone. Out of the energies computed in this way for varying $N_{\uparrow,\downarrow}$, the lowest gives the magnetization for the chosen values of N_p and U .

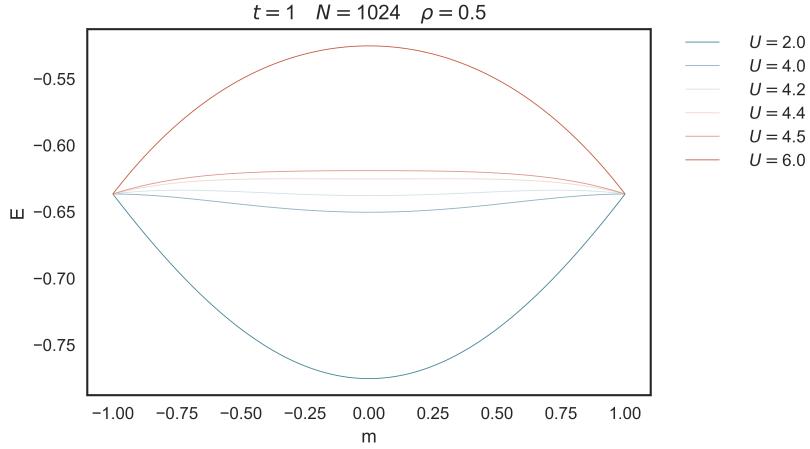


Figure 2.9: Mean field results at quarter filling for a 1024 sites chain. U is in units of t . As the on-site interaction is increased, we see a transition from a paramagnetic to a ferromagnetic phase.

Let us focus on figure (2.10). At $U = 2$, the phase is paramagnetic since the energy is minimized at $m = 0$. By $U = 4$, the phase transition is yet to occur but if you look at the energy scale in figure (2.9), you will see that the energy of the spin polarized solutions decreased dramatically. At $U = 4.2$, the large $|m|$ energies have turned down, although $m = 0$ is still the lowest energy solution. At $U = 4.4$, the phase transition occurs, and the solutions with $|m| = 1$ become the lowest energy solutions: we have reached the ferromagnetic phase.

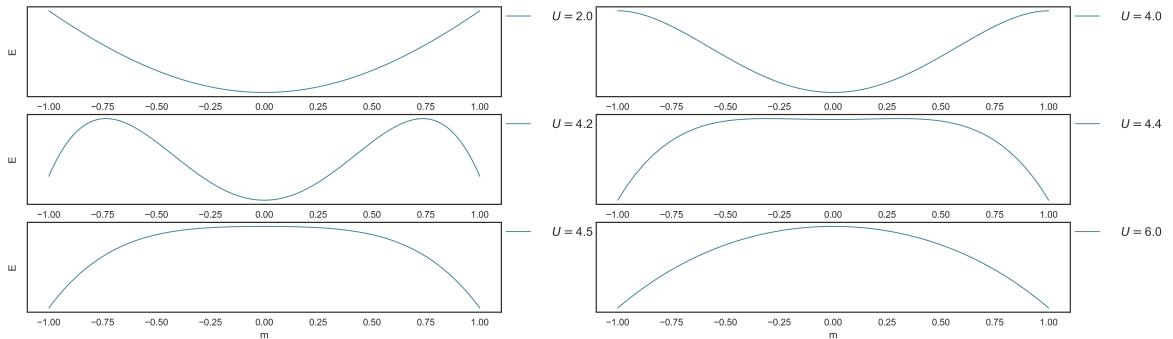


Figure 2.10: Plots of each energy curve separately giving evidence of a phase transition.

Are these results consistent with Stoner's criterion: $UN(\varepsilon_F) > 1$? First, we use the density of states obtained in section (2.3) to find a relation between the density ρ and the Fermi energy ε_F :

$$\rho(\varepsilon_F) = 2 \int_{-2t}^{\varepsilon_F} dE N(E) \rightsquigarrow \rho_{1D}(\varepsilon_F) = \frac{2}{\pi} \arccos \left(\frac{-\varepsilon_F}{2t} \right), \quad (2.85)$$

which behaves as expected, i.e. $\rho(-2t) = 0$, $\rho(0) = 1$, $\rho(2t) = 2$. In terms of the electron density:

$$N(\rho) = \frac{1}{2\pi t \sin(\pi\rho/2)}, \quad (2.86)$$

and in particular we can obtain the critical value U_c at which the transition to the ferromagnetic phase takes place. At quarter filling, we have $N(1/2) = 1/\sqrt{2}\pi t$, giving $U_c = \sqrt{2}\pi t \approx 4.44t$, which is about what we obtained at the mean field level⁸.

Mean field theory can be formulated in the GCE as well. One simply chooses the chemical potential μ , and then computes $N_{\uparrow,\downarrow}$ by filling the levels below μ . The density is changed by tuning μ . In the GCE case, the calculation is self-consistent, and is determined iteratively⁹: the densities are updated until convergence occurs. An example of the success of mean field is the discovery of striped phases of the Hubbard model, which are crucial in cuprate superconductors. Recently, these phases have been probed by the Quantum Monte Carlo (QMC) method we shall use in this thesis [82]. In fact, mean field theory is insightful, but uncontrolled. It tends to overestimate the possibility of ordering since it always predicts a phase transition. Even if the transition does occur, generally its details are not perfectly captured (the critical temperature, the critical exponents, ...).

2.6.3 Self-consistent solution in the GCE

In this section, we solve the mean field Hamiltonian in an iterative, self-consistent manner.

$$\mathcal{H}_{\text{MF}} = \mathcal{H}_{\uparrow} + \mathcal{H}_{\downarrow} + \mathcal{C}, \quad \mathcal{H}_{\sigma} = -t \sum_{\langle i,j \rangle} \left(c_{i,\sigma}^{\dagger} c_{j,\sigma} + c_{j,\sigma}^{\dagger} c_{i,\sigma} \right) + U \sum_i n_{i,\sigma} \langle n_{i,-\sigma} \rangle, \quad \mathcal{C} = -U \sum_i \langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle \quad (2.87)$$

Since the interacting problem is turned into a single particle problem, the solution basically consists of diagonalizing two $N \times N$ matrices, where N is the size of the system. By varying the $2N$ mean field parameters, which are essentially the average local densities $\langle n_{i,\sigma} \rangle$, we can find the ground state, or other excited states, at the mean field level. The mean field approach has several advantages: the Hilbert space is reduced from exponential to linear in the system size, which allows the study of relatively large systems; we can do the computation in real space; we can arbitrarily change the system geometry (introducing OBCs, defects, nonuniform hoppings); the model is flexible: tight-binding, and interaction terms are easily added to the Hamiltonian. However, $SU(2)$ symmetry is broken, and electron correlations are neglected. Only long range order is captured and its stability is often overestimated. While the mean field solution approaches the exact solution at weak coupling U , it can give only qualitative behavior at best, when U increases significantly.

The iterative method starts with the initialization of the mean field parameters. This initial condition cannot be completely arbitrary because it affects convergence. Typical choices are the random initial condition or the paramagnetic state.

Then, we repeat the following steps until convergence:

⁸Here, there can be finite size effects due to the finite size of the chain, $N = 1024$.

⁹One must pay attention so as not to get stuck in metastable states.

- Diagonalize \mathcal{H}_σ , obtaining the one-particle spectrum $\varepsilon_{\alpha,\sigma}$ and the corresponding eigenvectors.

$$\mathcal{H}_{\text{MF}} = \sum_{\alpha,\sigma} \varepsilon_{\alpha,\sigma} d_{\alpha,\sigma}^\dagger d_{\alpha,\sigma} + \mathcal{C}, \quad d_{\alpha,\sigma} = \sum_i Q_{\alpha i,\sigma}^* c_{i,\sigma} \quad (2.88)$$

- Recompute mean field parameters, and check for convergence: at iteration I , $\langle n_{i,\sigma} \rangle_I \approx \langle n_{i,\sigma} \rangle_{I-1}$.

$$\langle n_{i,\sigma} \rangle = \sum_{\alpha} |Q_{\alpha i,\sigma}|^2 (1 + e^{\beta(\varepsilon_{\alpha,\sigma} - \mu)})^{-1} \quad (2.89)$$

2.7 Simulatable variants of the Hubbard model

It is possible to think of more general models than the one considered so far. Notwithstanding, a limited basis of single-electron orbitals allows one to describe the essential electronic degrees of freedom. In fact, all the methodology we shall present in the next chapter generalizes for Hamiltonians belonging to a particular class [83]:

$$\mathcal{H} = - \sum_{i,j,\sigma} K_{ij} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + \sum_{i,j} V_{ij} n_i n_j, \quad (2.90)$$

where all the notation has the usual meaning, and V_{ij} , included in the functional of the charge density that models the Coulomb repulsion, already includes the effects of screening, and $n_i = c_{i,\uparrow}^\dagger c_{i,\uparrow} + c_{i,\downarrow}^\dagger c_{i,\downarrow}$.

This generic form includes standard condensed matter models, such as the Hubbard model, its multi-orbital, and extended variants, and the Anderson model. There is a huge variety of approximation methods at both zero and finite temperature devised specifically to study these models. We have seen some examples of such methods for the specific case of the Hubbard model. The methods aim at studying magnetism, superconductivity, and other low-temperature phase transitions perturbatively or by considering a simplified version of the model at hand. QMC methods follow a different route, allowing the exploration of a more vast range of parameter space. In auxiliary field QMC, the first step is to resort to a mathematical trick to eliminate the *direct* electron-electron interaction. In the same way that photon fields mediate the electromagnetic interaction, there are fields mediating our simplified screened interaction. In the context of a path integral formulation, we will introduce these so called Hubbard Stratonovich fields to eliminate the electron-electron interactions. The complexity of the problem is transferred to the degrees of freedom of the interaction of each electron with the external bosonic field that mediates their interactions. The problem of direct interactions between electrons maps to a free-fermion problem that can be solved formally in terms of determinants of single-electron Green's functions. While this problem still can't be solved analytically, we can devise a Monte Carlo method that uses importance sampling to probe the configuration space of the auxiliary bosonic fields.

The type of algorithms at hand tend to suffer from a number of difficulties, namely excessive computer time, the sign problem, fermionic wave functions turning bosonic, and numerical instabilities at low temperatures. We will discuss how some of these obstacles can be circumvented. With respect to the latter, a key, generic observation regarding thermodynamic studies of many-electron systems is in order. In the low temperature limit, the lowest energy states are assigned larger weights, whereas high

energy states are exponentially suppressed. However, Pauli's exclusion principle implies the existence of a "Fermi energy". The prevalent states are not macroscopically occupied, that is, they are only filled up to the "Fermi energy", which thus controls the physics of the system. Unfortunately, the information about the states around the Fermi energy is exponentially suppressed with respect to the comparatively unimportant states at the bottom of the band. Numerically, this translates into determining differences of large numbers with great precision. Finite-precision computers impose constraints on this process, but the limits can be stretched by using recently developed sophisticated algorithms. These explicitly separate the exponentially diverging numerical scales associated with the different energy scales (electron mobility, doping, Coulomb interaction, ...) with little extra computational cost. Thus, simulations can be stabilized at lower temperature, potentially allowing the study of more phases.

The case of interest for this work comes from considering a particular multi-orbital form of the very general Hamiltonian of Eq.(2.90). Even when inter-orbital interactions ($U' = 0$), yet is still numerically more expensive to simulate than the simple Hubbard model since the orbital space increases the overall dimensionality of the problem, and the hopping matrix is less sparse. Additional (greek) indexes are added to represent Wannier states on the same site, but corresponding to different "orbitals", and we consider interactions only between electrons on the same site and on the same orbital:

$$\mathcal{H} = - \sum_{\substack{x,y \\ \alpha,\beta,\sigma}} K_{(x\alpha)(y\beta)} \left(c_{x,\alpha,\sigma}^\dagger c_{y,\beta,\sigma} + c_{y,\beta,\sigma}^\dagger c_{x,\alpha,\sigma} \right) + \frac{U}{2} \sum_{\substack{x,\alpha \\ \sigma \neq \sigma'}} n_{x\alpha,\uparrow} n_{x\alpha,\downarrow} + \frac{U'}{2} \sum_{\substack{x,\alpha \neq \beta \\ \sigma,\sigma'}} n_{x\alpha,\sigma} n_{x\beta,\sigma'}, \quad (2.91)$$

While these models describe fundamentally different physics than the Hubbard model, they do not require a different formulation than the one used in simulations of the Hubbard model. This is easily seen by considering the change of variable $i = N_{\text{orb}}x + \alpha$, where N_{orb} is the number of orbitals in the model. It clearly collapses site and orbital indexes into the same index, bringing us back to a typical Hubbard-type model in a higher dimensional space. Additionally, the hopping matrix contains both the geometry, which specifies the structure of the class of materials, and potentially non-uniform transition amplitudes related to the specific one at hand. A general form for these in TMDs is derived by symmetry arguments in [50], and their specific values for different materials are obtained by fitting to the results of density functional theory (DFT), using the minimal model obtained by symmetry.

3

Auxiliary Field Quantum Monte Carlo

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We start with a brief review of the Monte Carlo method in statistical physics, and then explain how the fundamental concepts we present can be generalized to study quantum-many fermion systems. Focusing on the auxiliary field method, we discuss the mapping to the free-fermion problem that reduces the problem to the evaluation of determinants, and show how an efficient algorithm can be designed by successive global updates of the free-fermion Green's functions. Then, we explain how to control the instabilities in this update scheme. In particular, we explain how to circumvent low temperature instabilities due to the ill-conditioning of the matrices representing the free-fermion propagators. We also show that this problem has to do with the coexistence of significantly different energy scales, and tends to get worse as the size increases. Finally, we compute the estimators allowing the measurement of some relevant observables for Transition Metal Dichalcogenide Nanoribbons (TMDNRs).

3.1 Monte Carlo Method in Statistical Physics

Monte Carlo methods form the largest and arguably most useful class of numerical methods used to approach statistical physics problems. Statistical physics often deals with computing quantities that describe the behavior of condensed matter systems. The main difficulty one faces when doing so has to do with the collective nature of these systems. Many identical components comprise them, and while the equations that govern the behavior of the whole may be easy to write down, their solution is in general a remarkably laborious mathematical problem. It is both the sheer number of equations and the coupling between them that deems the task of finding an exact solution either very tough or even impossible. Concomitantly, the exponentially large number of possible configurations of the typical condensed matter system can be daunting. Thus, it is rather striking that we are able to describe a system that is governed by a macroscopically large number of equations in terms of only a few variables. The loss of information in doing so is only apparent.

The statistical description is so effective because most of the possible states of the system are extremely improbable when compared to the relevant very narrow part of configuration space. The success of the field is largely attributed to the averaging out that naturally occurs when measuring a property of a macroscopic system.

Suppose you try to sample uniformly from the probability distribution of all possible configurations of one of the aforementioned systems. Changes are your algorithm will not end before the Universe does. This is the computational complexity hurdle. A related issue is that of finite size effects. We are far from being able to simulate a macroscopically sized system. At best we can simulate a system that has only a minuscule fraction of the size of a real system. Amazingly there are techniques that allow us to efficiently extract information out of relatively small scale simulations. Nonetheless, increasing the system size systematically improves the reliability of a simulation. Thus, it is important to design efficient algorithms to probe larger systems in a fixed computer time frame.

The law of large numbers affords an approximation to integrals which can be written as an expectation of a random variable. Upon drawing enough independent samples from the corresponding distribution, the sample mean gets arbitrarily close to the integral at stake.

$$\mathbb{E}[f(X)] = \int dx f(x)p(x), \quad (3.1)$$

where $p(x)$ is the distribution of X .

We could simply draw M independent and identically distributed samples $x_{1,\dots,M}$ from $p(x)$ and approximate the integral as

$$\frac{1}{M} \sum_{k=1}^M f(x_k), \quad (3.2)$$

which in most cases converges to the desired expectation, as long as M is large enough. How large?

$$\text{Var}\left(\frac{1}{M} \sum_{k=1}^M f(x_k)\right) = \frac{1}{M} \text{Var}(f(x_1)) \propto \mathcal{O}\left(\frac{1}{M}\right) \quad (3.3)$$

Thus, the correction to the sample mean is of order $\mathcal{O}(\frac{1}{\sqrt{M}})$ as long as $\text{Var}(f(x_1)) \sim 1$, which can be achieved by using importance sampling, a variance reduction technique we will shortly discuss.

But how do we sample from an arbitrary distribution $p(X)$? The idea is to first make an educated choice of a Markov Chain with the prescribed stationary distribution from which we ultimately desire to sample from, $p(X)$. After a sufficiently high number of steps, a Markov Chain Monte Carlo (MCMC) algorithm generates samples from the target distribution. Imposing some conditions on this Markov Chain, namely that it should be irreducible, aperiodic and positive recurrent, the ergodic theorem guarantees that the empirical measures of the aforementioned sampler approach the target stationary distribution. Another important condition to impose on this Markov Chain is detailed balance. Let the transition matrix be $\mathbf{P} = [P_{\mu \rightarrow \nu}]$, and the state space Ω be $\{\pi_\mu | \mu = 1, \dots, |\Omega|\}$, where $|\Omega|$ is the total number of possible states. Then, the condition of detailed balance is defined for all μ, ν as

$$\pi_\mu P_{\mu \rightarrow \nu} = P_{\nu \rightarrow \mu} \pi_\nu \quad (3.4)$$

Consider a system in state μ that makes transitions to state ν at a rate $R_{\mu \rightarrow \nu}$ (that specifies the system's dynamics) and vice-versa. The probability that a system is in state μ at time t , $p_\mu(t)$, such that $\sum_\mu p_\mu(t) = 1$, is given by the master equation(s):

$$\frac{dp_\mu}{dt} = \sum_\nu [p_\nu(t)R_{\nu \rightarrow \mu} - p_\mu(t)R_{\mu \rightarrow \nu}] \quad \forall \mu \in \Omega \quad (3.5)$$

The equilibrium occupation probabilities at finite temperature T follow the Boltzmann distribution.

$$\pi_\mu = \lim_{t \rightarrow \infty} p_\mu(t) = \frac{1}{Z} e^{-E_\mu/k_B T}, \quad (3.6)$$

where E_μ is the energy of state μ , k_B is Boltzmann's constant, and Z is the partition function, from which we can extract thermodynamic functions in terms of expectations of physical quantities $\langle Q \rangle$, and response functions in terms of their variance σ_Q^2 .

Imposing the condition of stationarity on Eq.(3.5), $d_t p_\mu = 0$, and noting that $P_{\mu \rightarrow \nu} = R_{\mu \rightarrow \nu} dt$, we obtain the equilibrium condition

$$\sum_{\nu} \pi_{\mu} P_{\mu \rightarrow \nu} = \sum_{\nu} P_{\nu \rightarrow \mu} \pi_{\nu} \iff \pi_{\mu} \sum_{\nu} P_{\mu \rightarrow \nu} = \sum_{\nu} P_{\nu \rightarrow \mu} \pi_{\nu} \iff \pi_{\mu} = \sum_{\nu} P_{\nu \rightarrow \mu} \pi_{\nu} \quad (3.7)$$

This condition is enough to ensure convergence to an equilibrium of the dynamics of the Markov process. However, it does not guarantee that the reached distribution is our desired one, $\boldsymbol{\pi}$, after running the process for long enough. The probability of a state evolves according to

$$\pi_{\nu}(t+1) = \sum_{\mu} P_{\mu \rightarrow \nu} \pi_{\mu}(t) \iff \boldsymbol{\pi}(t+1) = \mathbf{P}\boldsymbol{\pi}(t) \quad (3.8)$$

The stationary distribution of a Markov chain obeys

$$\boldsymbol{\pi}(\infty) = \mathbf{P}\boldsymbol{\pi}(\infty), \quad (3.9)$$

however, condition (3.7) also allows for limit cycles of length n , where $\boldsymbol{\pi}$ rotates around a number of configurations:

$$\boldsymbol{\pi}(\infty) = \mathbf{P}^n \boldsymbol{\pi}(\infty), \quad (3.10)$$

where \mathbf{P}^n is the n-th power of \mathbf{P} .

Detailed balance is a stronger requirement than the equilibrium condition, which eliminates limit cycles, thus ensuring that our sampler draws configurations from the desired distribution. Intuitively, detailed balance corresponds to incorporating time-reversal symmetry in a simulation. The condition imposes a constraint on the Markov transition probabilities:

$$\frac{P_{\mu \rightarrow \nu}}{P_{\nu \rightarrow \mu}} = \frac{\pi_{\nu}}{\pi_{\mu}} = e^{-\beta(E_{\nu} - E_{\mu})} \quad (3.11)$$

Crucially, Monte Carlo methods employ *importance sampling*. It turns out that we can improve upon our estimate of $\mathbb{E}[f(X)]$ by reducing the variance of the estimator. If we introduce a separate distribution $q(x)$, and define a weight function as $w(x) = p(x)/q(x)$, we can rewrite equation (3.1):

$$\mathbb{E}[f(X)] = \int dx f(x) q(x) w(x) = \mathbb{E}[f(Y) w(Y)], \quad (3.12)$$

with $Y \sim q$, i.e. the random variable Y follows the distribution $q(Y)$.

It appears as though we didn't gain anything. However, by choosing q wisely, we can actually reduce the variance we computed in Eq.(3.3):

$$\text{Var}\left(\frac{1}{M} \sum_{k=1}^M f(y_k) w(y_k)\right) = \frac{1}{M} \text{Var}\left(f(y_1) w(y_1)\right) \quad (3.13)$$

Since we didn't make any assumptions about $q(Y)$, it may be chosen so as to minimize the variance, hence the error of the Monte Carlo estimator, improving the approximation of the expectation. However, note that the error remains proportional to $\frac{1}{\sqrt{M}}$. In practice, we devise a method to select

the portion of state space which contains states contributing more significantly to the average. This procedure ensures that $\text{Var}(f(y_1)w(y_1)) \sim 1$, improving the efficiency of our sampler. The choice of the weight function translates to the averaging process by changing the estimator. Explicitly computing the average

$$\langle Q \rangle = \frac{\sum_{\mu} Q_{\mu} e^{-\beta E_{\mu}}}{\sum_{\mu} e^{-\beta E_{\mu}}} \quad (3.14)$$

is only tractable for very small systems. In practice, we choose a subset of M states $\{\mu_1, \mu_2, \dots, \mu_M\}$, and estimate the average as

$$Q_M = \frac{\sum_{i=1}^M Q_{\mu_i} \pi_{\mu_i}^{-1} e^{-\beta E_{\mu_i}}}{\sum_{j=1}^M \pi_{\mu_j}^{-1} e^{-\beta E_{\mu_j}}} \quad (3.15)$$

The estimate improves as N increases, and when $N \rightarrow \infty$, $Q_M \rightarrow \langle Q \rangle$. The accuracy of the estimator depends on the choice of the probabilities $\boldsymbol{\pi}$, which is related to the aforementioned variance. For example, if $\boldsymbol{\pi}$ corresponds to the uniform distribution, i.e. $\pi_{\mu} = \frac{1}{|\Omega|} \forall \mu \in \Omega$, we have

$$Q_M = \frac{\sum_{i=1}^M Q_{\mu_i} e^{-\beta E_{\mu_i}}}{\sum_{j=1}^M e^{-\beta E_{\mu_j}}}, \quad (3.16)$$

which turns out to be a poor choice since most of the visited states contribute negligibly to the average, leading to an inaccurate estimate. The sum is dominated by a small subset of states, which we would like to access. The idea of the Quantum (Classical) Monte Carlo method is to simulate the random quantum (thermal) fluctuations of a system, as it oscillates between states in a given time frame [84]. Instead of visiting these states uniformly, the most relevant part of the phase space is sampled more frequently, overcoming the seemingly exponential complexity of computing a sample mean numerically. Even though only a small fraction of the system's states are sampled, we then obtain an accurate estimate of physical quantities of interest, namely energy, and correlation functions. This is implemented via a proposal-acceptance scheme.

To exploit the freedom given by condition (3.11), we note that we can always introduce a non-zero “stay-at-home” probability $P_{\mu \rightarrow \mu} \in [0, 1]$. Regardless of its value, detailed balance is satisfied. Similarly, any adjustment in $P_{\mu \rightarrow \nu}$ must be compensated by changing $P_{\nu \rightarrow \mu}$ to preserve their ratio. Break the transition probability into a selection probability and an acceptance ratio, respectively:

$$\frac{P_{\mu \rightarrow \nu}}{P_{\nu \rightarrow \mu}} = \frac{S_{\mu \rightarrow \nu} A_{\mu \rightarrow \nu}}{S_{\nu \rightarrow \mu} A_{\nu \rightarrow \mu}} \quad (3.17)$$

The Markov process now consists of generating a chain of states according to $S_{\mu \rightarrow \nu}$, which are then accepted or rejected depending on $A_{\mu \rightarrow \nu}$. Since we want to make the algorithm as efficient as possible, we want to make the acceptance ratio as close to one as possible to avoid useless steps. The most common way to do this is to fix the largest of them to one, and adjust the other accordingly. The acceptance ratio will be close to one more often if $S_{\mu \rightarrow \nu}$ includes most of the dependence of $P_{\mu \rightarrow \nu}$ on the characteristics of the states μ, ν . Ideally, states would always be selected with the correct transition probability, and the acceptance ratio would be fixed to unity. Good algorithms approach this situation,

and much effort has been directed at optimizing them to do so. By far, the most common sampling scheme choice is the Metropolis-Hastings algorithm, which we now describe.

We select the transition probability to be uniform, and impose detailed balance through the choice of the acceptance ratios:

$$\frac{P_{\mu \rightarrow \nu}}{P_{\nu \rightarrow \mu}} = \frac{A_{\mu \rightarrow \nu}}{A_{\nu \rightarrow \mu}} = e^{-\beta(E_\nu - E_\mu)} \quad (3.18)$$

Suppose that $E_\mu < E_\nu$. Then, $A(\nu \rightarrow \mu) > A(\mu \rightarrow \nu)$, and since only the acceptance ratio is fixed, we may freely set $A(\nu \rightarrow \mu) = 1$, which fixes $A(\mu \rightarrow \nu) = e^{-\beta(E_\nu - E_\mu)}$. This choice maximizes the efficiency of the algorithm. In short, we propose a random new state uniformly, and then we accept it with probability $A_{\mu \rightarrow \nu} = \min(1, e^{-\beta(E_\nu - E_\mu)})$.

Before we can use the states generated by our sampler to measure averages of physical quantities, we must reach the stationary distribution of the Markov process. We consider this condition to be satisfied after a time τ_{eq} , measured in steps of the algorithm. When we consider a lattice model with a discrete set of states at each site $i = 1, 2, \dots, N$, we say that a *sweep* is completed whenever N Monte Carlo steps are performed. Thus, the number of “warm-up” sweeps is of order $W \sim \tau_{\text{eq}}/N$.

Before running a simulation, we need to decide how many sweeps we need to get an accurate estimate of the average. The problem is that we need uncorrelated samples to average over. To clarify, let us choose a specific model. The paradigmatic model of statistical physics is the Ising model, a classical model of a magnet, which consists of considering spins-1/2 on a lattice, interacting only with their nearest neighbors. Since each spin can only take on two values, say ± 1 , there are 2^N possible states. The Hamiltonian reads

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - B \sum_i s_i, \quad (3.19)$$

where $\langle i,j \rangle$ means that i, j are nearest neighbors on the lattice.

A simple strategy to sample configurations of the Ising model is single-spin-flip dynamics. We start with a random configuration of the spins, and then propose new configurations at each step by flipping a single spin at a given site. A sweep is completed after we propose a spin flip at every site on the lattice.

Consecutive configurations generated by this chain differ only slightly. Thus, it takes some time for the system to reach a configuration which is significantly different from the initial one. This characteristic time is called the correlation time τ_c . A rigorous manner to estimate τ_c is through the time-displaced auto-correlation function associated to some quantity being measured. An example of a relevant quantity for the case of the Ising model is the magnetization per site:

$$m = \frac{1}{N} \sum_i s_i \quad (3.20)$$

Its associated time-displaced auto-correlation is

$$\chi_m(t) = \int dt' \left(m(t') - \langle m \rangle \right) \left(m(t'+t) - \langle m \rangle \right) = \int dt' \left(m(t')m(t'+t) - \langle m \rangle^2 \right) \quad (3.21)$$

giving a measure of how correlated two measurements of the magnetization separated by a simulation time t are.

The typical time-scale on which $\chi_m(t)$ falls off is a measure of the correlation time of the simulation. In particular, at long times it falls off exponentially. The definition of τ_c stems from this characteristic long-time behavior: $\chi_m(t) \sim e^{-t/\tau_c}$. In practice, after waiting for $2\tau_c$, the measurements are virtually uncorrelated. Let A be the number of sweeps roughly corresponding to $2\tau_c$ steps. Then, if we make S sweeps of the lattice during the simulation, the number of independent measurements (i.e. with A sweeps between them) is

$$M = \frac{S - W}{A} \quad (3.22)$$

There are many ways to estimate τ_c from $\chi_m(t)$. The simplest consists of making an exponential fit in a given range of times. However, this might be unreliable since the estimate depends strongly on the chosen range. An alternative is to compute the “integrated” correlation time:

$$\int_0^\infty dt \frac{\chi_m(t)}{\chi_m(0)} = \int_0^\infty dt e^{-t/\tau_c} = \tau_c, \quad (3.23)$$

which is less sensitive, but not perfect either since the error that is introduced when the assumption that “long-time” behavior has been reached is arbitrary and introduces an uncontrolled error. Moreover, the very long-time behavior of the auto-correlation is rather noisy and must be excluded.

Using measured data for the magnetization at evenly-spaced times, we may construct the time-displaced auto-correlation function up to an unimportant constant, which does not affect the estimate of the correlation time:

$$\chi_m(t) = \frac{1}{t_{\max} - t} \sum_{t'=0}^{t_{\max}-t} m(t')m(t'+t) - \frac{1}{t_{\max} - t} \sum_{t'=0}^{t_{\max}-t} m(t') \frac{1}{t_{\max} - t} \sum_{t'=0}^{t_{\max}-t} m(t'+t), \quad (3.24)$$

where t_{\max} is the total simulation time in MC steps.

One should be careful when using this expression at very long times. As t approaches t_{\max} , the upper limit of the sums decreases, and the integration interval becomes narrower. Since $m(t)$ fluctuates randomly at very long times, the statistical error associated to $\chi_m(t)$ becomes more prominent as t approaches t_{\max} . This turns out not to be problematic since typical simulations run for many correlation times. Thus, the tails of the auto-correlation may safely be neglected because the correlations will have already vanished, by definition.

To finish our discussion on the issue of computing the time-displaced correlator, we note that if we have a total of N_s samples of, for instance, magnetization data, the complexity of computing χ_m is $\mathcal{O}(N_s^2)$. It is possible to speed up this process by computing its Fourier transform $\tilde{\chi}_m(\omega)$, and

inverting to recover $\chi_m(t)$. This can be done via a standard Fast Fourier Transform (FFT) algorithm in $\mathcal{O}(2N_s \log N_s)$ flops. To do this, we apply the following trick

$$\begin{aligned}\tilde{\chi}_m(\omega) &= \int dt e^{i\omega t} \int dt' \left(m(t') - \langle m \rangle \right) \left(m(t' + t) - \langle m \rangle \right) \\ &= \int dt \int dt' e^{-i\omega t'} \left(m(t') - \langle m \rangle \right) e^{i\omega(t'+t)} \left(m(t' + t) - \langle m \rangle \right) = \tilde{m}'(\omega) \tilde{m}'(-\omega) = |\tilde{m}'(\omega)|^2,\end{aligned}\tag{3.25}$$

where $\tilde{m}'(\omega)$ is the Fourier transform of $m'(t) = m(t) - \langle m \rangle$ ¹.

In practice, when implementing a MC algorithm, we take a measurement say every sweep (which can be less than a correlation time), and then compute the time-displaced correlator at the end of the simulation to estimate the correlation time. How can we estimate the error in the mean of the N_s correlated samples without knowing τ_c in advance? Take again magnetization measurements. Suppose your N_s samples were independent. The standard deviation of their mean would be well known:

$$\sigma = \sqrt{\frac{\frac{1}{N_s} \sum_{i=0}^{N_s-1} (m_i - \bar{m})^2}{N_s - 1}} = \sqrt{\frac{1}{N_s - 1} (\bar{m}^2 - \bar{m}^2)}\tag{3.26}$$

Intuitively, to get the correct result, we could simply replace N_s by M , as computed in Eq.(3.22), in the last step. This is because the mean shouldn't change very much when including the correlated configurations with nearly the same magnetization. However, the number of uncorrelated samples is certainly smaller than N_s , and can be estimated to be M by auto-correlation studies.

As shown in [85], if the samples are separated by a time interval Δt , the correct expression is

$$\sigma = \sqrt{\frac{1 + 2\tau_c/\Delta t}{N_s - 1} (\bar{m}^2 - \bar{m}^2)},\tag{3.27}$$

which reduces to Eq.(3.26) when $\Delta t \gg \tau_c$, since in that case the samples are virtually uncorrelated. Also, we now have a rigorous justification for estimating the amount of time between uncorrelated samples as $2\tau_c$, since for much longer times, the samples become uncorrelated.

Often, we work with heavily correlated samples, so that instead we have $\Delta t \ll \tau_c$. In this limit, the 1 in the numerator of Eq.(3.27) can be neglected, and noting that the number of sweeps between measurements corresponding to Δt is $\Delta S = (S - W)/N_s$, we have

$$\sigma \approx \sqrt{\frac{A}{S - W} (\bar{m}^2 - \bar{m}^2)},\tag{3.28}$$

the same result we would obtain by simply replacing N_s by M . What we found, in rigorous terms, was that the presence of many correlated samples does not significantly change the sample mean if $\Delta t \ll \tau_c$. If we take enough correlated samples, their influence on the sample mean averages out.

Eq.(3.28) has the advantage of being independent of Δt , which allows us to choose Δt freely, without affecting the final error. This is handy since it allows us to choose Δt small so as not to lose data.

¹The only difference between $\tilde{m}'(\omega)$ and $\tilde{m}(\omega)$, is that $\tilde{m}'(0) = 0$, while $\tilde{m}(0) \neq 0$. Thus, one can also compute $\tilde{m}(\omega)$ and then set its $\omega = 0$ component to zero.

3.2 Theoretical Framework and Mathematical Formulation

Auxiliary-field, or Determinant QMC is a simulation method that is commonly used to simulate the Hubbard model, allowing one to capture the elusive effects of electron correlations in the two-dimensional graphene-like nanostructures we are concerned with. The sign problem may deem the algorithm exponentially complex in the size of the system and in inverse temperature, but it is possible to overcome this hurdle for a class of models, namely the Hubbard model on a bipartite lattice at half filling ($\mu = 0$ in our conventions). In fact, many interesting phenomena occur at half filling, for example magnetic ordering and the Mott metal-insulator transition. The difficulty lies in computing the nearly vanishing average of a random variable X with comparatively large variance, i.e. $\sigma_X / \langle X \rangle \gg 1$.

Ultimately, we seek a computable approximation of the projection operator \mathcal{P} defined in equation (2.20). As we shall see, it is found by using (either a discrete or continuous) Hubbard-Stratonovich transformation. This transformation introduces an auxiliary field (consisting basically of Ising spins), and we use Monte Carlo to sample configurations from the distribution corresponding to this *classical* configuration space. This approach is equivalent to an exact solution of the mean field problem, an observation which motivates us to compare our results with the mean field ones.

Mean field theory may be formulated by applying the Hubbard Stratonovich (HS) transformation to transform an interacting problem into a one-body problem, and then apply the saddle-point approximation to solve the resulting integrals. In the Grand-canonical ensemble (GCE) (where we make $\mathcal{H} \mapsto \mathcal{H} - \mu\mathcal{N}$, \mathcal{N} being the total particle number), the partition function may be written in terms of a functional integral² over a space-time dependent field of the exponential of a one-body action

$$Z = \text{Tr}[e^{-\beta\mathcal{H}}] = \int \mathcal{D}\mathbf{h} e^{-S(\mathbf{h})} \equiv \text{Tr}_{\mathbf{h}}[e^{-S(\mathbf{h})}], \quad (3.29)$$

which may be computed by Monte Carlo sampling. In mean field, we approximate the integral by replacing the functional integral by a constant times the exponential action itself evaluated at a single field \mathbf{h}^* , for which the action has a minimum: $\partial_{\mathbf{h}} S(\mathbf{h})|_{\mathbf{h}=\mathbf{h}^*} = 0$, and $\partial_{\mathbf{h}}^2 S(\mathbf{h})|_{\mathbf{h}=\mathbf{h}^*} > 0$.

The integral is evaluated exactly in the auxiliary field QMC method, which avoids the bias introduced by the specific choice of the HS decoupling. The nature of the analytical mean field solution depends on this choice, while the unbiased QMC solution does not, relying on a numerical solution that scales with the cubic volume of the system, and linearly with inverse temperature.

The sign problem may be seen as an inherent difficulty that arises from taking all possible fluctuations around the mean field solution. An advantage of determinant QMC is that certain symmetries of the model at hand, such as PHS in the Hubbard model, may be used to avoid the sign problem.

3.2.1 Trotter-Suzuki Decomposition

In section 2.3, we found exact solutions for particular instances of the Hubbard model by finding a closed form for the partition function [56]. When devising a numerical method, a good sanity check is

²In the case of a discrete HS transformation, as the one we shall use in what follows, we actually have a sum instead of a functional integral. We use the notation Tr to refer to both cases depending on the context.

to verify that it satisfactorily approximates the partition function since it is the quantity that can be used to obtain any observable. Computing the partition function of a quantum system in equilibrium

$$Z_\beta = \text{Tr}[e^{-\beta\mathcal{H}}] = \sum_{\alpha} \langle \psi_\alpha | e^{-\beta\mathcal{H}} | \psi_\alpha \rangle \quad (3.30)$$

is equivalent to studying its *imaginary* time evolution. The inverse temperature β represents the imaginary time $\tau = it$, and Z_β may be simply thought of as the wave function of the analogous quantum system at imaginary time β . In fact, for a zero temperature system, projective methods use this same principle to find the ground state. In that case, the partition function strictly corresponds to the ground state wave function when $\tau \rightarrow \infty$ (in practice, one takes $\tau = \Theta$ large enough).

Eq.(3.30) is not very amenable to numerical computation since it contains an exponential of a sum of non-commuting operators $e^{-\beta(\mathcal{H}_K + \mathcal{H}_V)}$ as per Eq.(2.18). The exponential is not factorizable and involves computing an infinite number of commutators containing these two operators, as per the Zassenhaus formula, valid for any two generic operators X and Y ³:

$$e^{\delta(X+Y)} = e^{\delta X} e^{\delta Y} e^{-\frac{\delta^2}{2}[X,Y]} e^{\frac{\delta^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])} e^{-\frac{\delta^4}{24}([[[X,Y],X],X]+3[[[X,Y],X],Y]+3[[[X,Y],Y],Y])} \dots, \quad (3.31)$$

where $\delta \in \mathbb{C}$ is an expansion parameter. The Trotter-Suzuki decomposition leads to the sought approximate factorization that is used to approximate the partition function. Dividing the imaginary time interval $[0, \beta]$ into L equal sub-intervals of small width $\Delta\tau = \beta/L$:

$$Z = \text{Tr} \left[\prod_{l=0}^{L-1} e^{-\Delta\tau\mathcal{H}} \right], \quad (3.32)$$

we obtain a form that is more amenable to computation. Actually, it also arises naturally by writing the matrix elements of the projection operator \mathcal{P} as path integrals (here, time ordering is implicit [4]):

$$\langle \psi | e^{-\beta\mathcal{H}} | \psi' \rangle = \sum_{|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_{L-1}\rangle} \langle \psi | e^{-\Delta\tau\mathcal{H}} | \psi_1 \rangle \langle \psi_1 | e^{-\Delta\tau\mathcal{H}} | \psi_2 \rangle \dots \langle \psi_{L-1} | e^{-\Delta\tau\mathcal{H}} | \psi' \rangle \quad (3.33)$$

Then, the partition function only selects paths that are periodic in imaginary time:

$$Z = \text{Tr}[e^{-\beta\mathcal{H}}] = \sum_{|\psi_0\rangle} \langle \psi_0 | e^{-\beta\mathcal{H}} | \psi_0 \rangle = \sum_{\{|\psi_l\rangle\}} \prod_{l=0}^{L-1} \langle \psi_l | e^{-\Delta\tau\mathcal{H}} | \psi_{l+1} \rangle \delta_{0,L} = \text{Tr} \left[\prod_{l=0}^{L-1} e^{-\Delta\tau\mathcal{H}} \right], \quad (3.34)$$

where we have $|\psi_L\rangle = |\psi_0\rangle$, and we recover the result of Eq.(3.32) by simply reorganizing the summations over $\{|\psi_l\rangle\}$, so as to make appear closure relations, resulting in unit operators in the Hilbert space of each slice. The “Trotter breakup” follows from truncating Eq.(3.31), and keeping only the first order term in $\Delta\tau$. In the $\Delta\tau \rightarrow 0$ limit, it becomes a trace of a time ordered exponential of the integral of the time-dependent action. The slice index l , or the argument τ , imply time ordering.

³This is just the inverse of the well known Baker–Campbell–Hausdorff formula commonly used in quantum mechanics.

$$Z = \text{Tr} \left[\prod_{l=0}^{L-1} e^{-\Delta\tau \mathcal{H}_K^l} e^{-\Delta\tau \mathcal{H}_V^l} \right] + \mathcal{O}(\Delta\tau^2) \xrightarrow{\Delta\tau \rightarrow 0} \text{Tr} \left[\mathcal{T}_\tau \exp \left(- \int_0^\beta d\tau \underbrace{(\mathcal{H}_K(\tau) + \mathcal{H}_V(\tau))}_{S(\tau)} \right) \right] \quad (3.35)$$

3.2.2 Hubbard-Stratonovich transformation

The kinetic energy term is quadratic in the fermion operators, and is spin-independent and thus may be separated into spin up and spin down components, independent of the time slice, i.e. $\mathcal{H}_{K_\sigma}^l = \mathcal{H}_{K_\sigma}$.

$$e^{-\Delta\tau \mathcal{H}_K} = e^{-\Delta\tau \mathcal{H}_{K\uparrow}} e^{-\Delta\tau \mathcal{H}_{K\downarrow}}, \quad (3.36)$$

where $\mathcal{H}_{K_\sigma} = \mathbf{c}_\sigma^\dagger (-t_\sigma \mathbf{K}_\sigma - \mu_\sigma \mathbf{I}) \mathbf{c}_\sigma$, and we allow spin-dependent hoppings and chemical potential.

The potential energy term, however, is quartic. Fortunately, it is possible to express it in quadratic form by introducing an extra degree of freedom, the so called *Hubbard-Stratonovich (HS) field* $\mathbf{h} \equiv (h_{l,i})_{i=0, l=0}^{N-1, L-1}$, in which each element is essentially an Ising spin. At each slice, the interaction is eliminated by an N -dimensional HS field $\tilde{\mathbf{h}}$. We start by noting that $[n_i, n_j] = 0 \forall i, j$, so that

$$e^{-\Delta\tau \mathcal{H}_V} = e^{-U \Delta\tau \sum_{i=1}^N (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)} = \prod_i e^{-U \Delta\tau (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)} \quad (3.37)$$

The HS transformation is based on the well known identity $e^{\frac{a^2}{2}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{z^2}{2}-za} dz \forall a > 0$, which is also valid for an operator \mathcal{A} , that is, making $a \mapsto \mathcal{A}$ in the Gaussian integral identity. Noting that $(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) = -\frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})^2 + \frac{1}{4}$, we can recast the potential energy term as

$$e^{-\Delta\tau \mathcal{H}_V} = \prod_i e^{\frac{U\Delta\tau}{2}(n_{i\uparrow} - n_{i\downarrow})^2} e^{-\frac{U\Delta\tau}{4}} = \left(\frac{\Delta\tau e^{-\frac{U\Delta\tau}{2}}}{\pi} \right)^{N/2} \int_{-\infty}^{\infty} \prod_i d\tilde{h}_i e^{-\Delta\tau [\tilde{h}_i^2 + \sqrt{2U}(n_{i\uparrow} - n_{i\downarrow})\tilde{h}_i]}, \quad (3.38)$$

so that in the $\tau \rightarrow 0$ limit, the partition function becomes

$$Z \propto \int \mathcal{D}\tilde{\mathbf{h}}(\tau) e^{-\int_0^\beta d\tau \tilde{\mathbf{h}}^2(\tau)} \text{Tr} \left[\mathcal{T}_\tau e^{-\int_0^\beta d\tau [\mathcal{H}_K(\tau) + \sqrt{2U}(\mathbf{n}_{\uparrow}(\tau) - \mathbf{n}_{\downarrow}(\tau)) \cdot \tilde{\mathbf{h}}(\tau)]} \right], \quad (3.39)$$

representing a system of noninteracting fermions coupled via spin to an external fluctuating real field.

The fact that $n_{i,\sigma}$ can only take on two possible values suggests an analogous transformation in which the fluctuating field can only take on two possible values. An Ising spin will prove sufficient to eliminate the direct electron-electron interaction.

A discrete HS transformation for $U > 0$ allows us to recast Eq.(3.37) in terms of the local spin, a non-interacting quadratic term $n_{i\uparrow} - n_{i\downarrow}$ (at each imaginary-time slice, since the operators live on the Hilbert space of that specific slice). Let $c_U = \frac{1}{2} e^{-\frac{U\Delta\tau}{4}}$ and $\nu = \text{arcosh}(e^{\frac{U\Delta\tau}{2}})$. Then, the sought transformation reads

$$e^{-U \Delta\tau (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)} = c_U \sum_{\tilde{h}_i=\pm 1} e^{\nu \tilde{h}_i (n_{i\uparrow} - n_{i\downarrow})} \quad (3.40)$$

Notice that $\Delta\tau$ appears explicitly in the coupling constant. This is because we worked with fixed

length Ising spins. In the Gaussian formulation we started with, $\Delta\tau$ can be reabsorbed in the HS field, even though $\Delta\tau$ is still implicit in the integration measure. The parameter $\frac{1}{\Delta\tau}$ can be seen as a high energy cutoff, and it must be larger than all other energy scales in the problem, which is required to make the Trotter breakup error small when discretizing time onto a lattice of $L = \beta/\Delta\tau$ points.

To prove Eq.(3.40), let us write down how the operators $(n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$ and $(n_{i\uparrow} - n_{i\downarrow})$ act on a state on a given site.

$$(n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \begin{cases} | \rangle = \frac{1}{4} | \rangle \\ |\uparrow\rangle = -\frac{1}{4} |\uparrow\rangle \\ |\downarrow\rangle = -\frac{1}{4} |\downarrow\rangle \\ |\uparrow\downarrow\rangle = \frac{1}{4} |\uparrow\downarrow\rangle \end{cases} \quad (n_{i\uparrow} - n_{i\downarrow}) \begin{cases} | \rangle = 0 | \rangle \\ |\uparrow\rangle = |\uparrow\rangle \\ |\downarrow\rangle = |\downarrow\rangle \\ |\uparrow\downarrow\rangle = 0 |\uparrow\downarrow\rangle \end{cases} \quad (3.41)$$

We can now compare the action of the operators on the LHS and on the RHS of Eq.(3.40) and find the desired relation by defining $\cosh \nu = \frac{1}{2}(e^\nu + e^{-\nu}) \equiv e^{\frac{U\Delta\tau}{2}}$.

$$\begin{aligned} e^{-U\Delta\tau(n_{i\uparrow}-1/2)(n_{i\downarrow}-1/2)} |\psi\rangle &= e^{-\frac{U\Delta\tau}{4}} |\psi\rangle, |\psi\rangle = | \rangle, |\uparrow\downarrow\rangle \\ e^{-U\Delta\tau(n_{i\uparrow}-1/2)(n_{i\downarrow}-1/2)} |\uparrow(\downarrow)\rangle &= e^{\frac{U\Delta\tau}{4}} |\uparrow(\downarrow)\rangle \\ c_U \sum_{\tilde{h}_i=\pm 1} e^{\nu \tilde{h}_i(n_{i\uparrow}-n_{i\downarrow})} |\psi\rangle &= e^{-\frac{U\Delta\tau}{4}} |\psi\rangle, |\psi\rangle = | \rangle, |\uparrow\downarrow\rangle \\ c_U \sum_{\tilde{h}_i=\pm 1} e^{\nu \tilde{h}_i(n_{i\uparrow}-n_{i\downarrow})} |\uparrow(\downarrow)\rangle &= \frac{e^\nu + e^{-\nu}}{2} e^{-\frac{U\Delta\tau}{4}} |\uparrow(\downarrow)\rangle \end{aligned} \quad (3.42)$$

Note that we require $U > 0$ so that there exists $\nu \in \mathbb{R}$ such that $\cosh \nu = e^{U\Delta\tau/2}$. A similar reasoning could be made for $U < 0$. Similar transformations that recast other types of quartic terms in terms of quadratic ones exist, but we shall not need them in what follows [8]. The transformation we derived is the one we will use throughout. We have made progress at the expense of introducing L fields $\tilde{\mathbf{h}}$ to each fermions are coupled to at each slice. More precisely, the external field couples to the local spin at each site. Our representation of the interacting problem is *exact*, and is encoded in the configurations of the NL -dimensional HS field \mathbf{h} [56].

The interacting term

$$e^{-\Delta\tau \mathcal{H}_V} = \prod_{i=0}^{N-1} \left(c_U \sum_{\tilde{h}_i=\pm 1} e^{\nu \tilde{h}_i(n_{i\uparrow}-n_{i\downarrow})} \right), \quad (3.43)$$

can be manipulated to arrive at a more compact form.

$$\begin{aligned} e^{-\Delta\tau \mathcal{H}_V} &= (c_U)^N \sum_{\tilde{h}_0=\pm 1} e^{\nu \tilde{h}_0(n_{0\uparrow}-n_{0\downarrow})} \sum_{\tilde{h}_1=\pm 1} e^{\nu \tilde{h}_1(n_{1\uparrow}-n_{1\downarrow})} \dots \sum_{\tilde{h}_{N-1}=\pm 1} e^{\nu \tilde{h}_{N-1}(n_{N-1\uparrow}-n_{N-1\downarrow})} \\ &= (c_U)^N \sum_{\{\tilde{h}_i=\pm 1\}} e^{\sum_{i=0}^{N-1} [\nu \tilde{h}_i(n_{i\uparrow}-n_{i\downarrow})]} \equiv (c_U)^N \text{Tr}_{\tilde{\mathbf{h}}} \left[e^{\sum_{i=0}^{N-1} [\nu \tilde{h}_i(n_{i\uparrow}-n_{i\downarrow})]} \right] \\ &= (c_U)^N \text{Tr}_{\tilde{\mathbf{h}}} \left[e^{\sum_{i=0}^{N-1} \nu \tilde{h}_i n_{i\uparrow}} e^{-\sum_{i=0}^{N-1} \nu \tilde{h}_i n_{i\downarrow}} \right] = (c_U)^N \text{Tr}_{\tilde{\mathbf{h}}} \left[e^{\mathcal{H}_{V\uparrow}} e^{\mathcal{H}_{V\downarrow}} \right], \end{aligned} \quad (3.44)$$

where the spin up and spin down operators \mathcal{H}_{V_σ} are defined as follows

$$\mathcal{H}_{V\sigma} = \sum_{i=0}^{N-1} \nu \tilde{h}_i n_{i\sigma} = \sigma \nu \mathbf{c}_\sigma^\dagger \mathbf{V}(\tilde{\mathbf{h}}) \mathbf{c}_\sigma, \quad (3.45)$$

with $\mathbf{V}(\tilde{\mathbf{h}})$ being simply the HS-field put into a diagonal $N \times N$ matrix: $\mathbf{V}(\tilde{\mathbf{h}}) \equiv \text{diag}(\tilde{h}_0, \tilde{h}_1, \dots, \tilde{h}_{N-1})$.

3.2.3 Single-particle propagators and the fermionic trace

For each imaginary time slice l , we may define a HS-field $\tilde{\mathbf{h}}_l$, which in turn specifies \mathbf{V}_l and $\mathcal{H}_{V_\sigma}^l$. Note that the Hamiltonian has acquired a “fictitious” imaginary-time dependence that merely serves to enforce (imaginary-)time ordering, and independent Hilbert spaces at each slice. We may now replace the result of equation (3.44) in equation (3.35), and exchange the traces to obtain

$$Z = (c_U)^{NL} \text{Tr}_{\mathbf{h}} \text{Tr} \left[\prod_{l=0}^{L-1} \underbrace{\left(e^{-\Delta\tau \mathcal{H}_{K\uparrow}} e^{\mathcal{H}_{V\uparrow}^l} \right)}_{B_{l,\uparrow}(\tilde{\mathbf{h}}_l)} \underbrace{\left(e^{-\Delta\tau \mathcal{H}_{K\downarrow}} e^{\mathcal{H}_{V\downarrow}^l} \right)}_{B_{l,\downarrow}(\tilde{\mathbf{h}}_l)} \right], \quad (3.46)$$

where all operators are now quadratic in the fermion operators:

$$\mathcal{H}_{K_\sigma} = \mathbf{c}_\sigma^\dagger (-t_\sigma \mathbf{K}_\sigma - \mu_\sigma \mathbf{I}) \mathbf{c}_\sigma \quad \mathcal{H}_{V_\sigma}^l = \sigma \nu \mathbf{c}_\sigma^\dagger \mathbf{V}_l(\tilde{\mathbf{h}}_l) \mathbf{c}_\sigma \quad (3.47)$$

for $\sigma = \pm 1$ and $\mathbf{V}_l(\tilde{\mathbf{h}}_l) = \text{diag}(h_{l,0}, h_{l,1}, \dots, h_{l,N-1})$.

Furthermore, we have defined the \mathbf{B} -matrices, representing the imaginary-time propagators between time slices.

$$\mathbf{B}_{l,\sigma}(\tilde{\mathbf{h}}_l) = e^{\Delta\tau(t_\sigma \mathbf{K}_\sigma + \mu_\sigma \mathbf{I})} e^{\sigma \nu \mathbf{V}_l(\tilde{\mathbf{h}}_l)} \quad (3.48)$$

The problem of computing the partition function has been reduced to computing the trace of a product of exponentials of quadratic forms. Thus, we may still rewrite equation (3.46) by making use of the following identity.

Let \mathcal{H}_l be quadratic forms of the fermion operators:

$$\mathcal{H}_l = c_i^\dagger (\mathbf{H}_l)_{ij} c_j, \quad (3.49)$$

where the summation is implied, and where \mathbf{H}_l are real matrices. Then, the following identity holds

$$\text{Tr} [e^{-\mathcal{H}_1} e^{-\mathcal{H}_2} \dots e^{-\mathcal{H}_L}] = \det(\mathbf{I} + e^{-\mathbf{H}_L} e^{-\mathbf{H}_{L-1}} \dots e^{-\mathbf{H}_1}) \quad (3.50)$$

For simplicity, in appendix B, we present the proof for a simpler case, corresponding to a single \mathbf{B} -matrix, i.e. a product of exponentials of two quadratic operators [7]. It could then be easily extended to the more general case [83](ch.4, ap. III). The products of up and down spin \mathbf{B} -matrices give rise to a product of two such determinants, which may easily be deduced from the proof of appendix B.

When applied to our problem, Eq.(3.50) essentially makes the computation of the trace possible! Note that if we were to compute it naively, we would soon run out of computer memory. The dimension

of the Hilbert space of the Hubbard model is exponential in the number of sites N (actually 4^N). At worst, the determinant can be calculated in $\mathcal{O}(N^3)$ flops for a matrix whose size is polynomial in N , leading to a naive $\mathcal{O}(N^4)$ algorithm. The computable form of the partition function (3.46) is

$$Z = \text{Tr}_{\mathbf{h}} \left[(c_U)^{NL} \det[\mathbf{M}_\uparrow(\mathbf{h})] \det[\mathbf{M}_\downarrow(\mathbf{h})] \right] = \sum_{\{\mathbf{h}\}} P(\mathbf{h}) \equiv \text{Tr}_{\mathbf{h}} [e^{-S(\mathbf{h})}] \quad (3.51)$$

where the fermion matrices \mathbf{M}_σ are defined in terms of the \mathbf{B} -matrices that depend on the HS-field \mathbf{h} :

$$\mathbf{M}_\sigma(\mathbf{h}) = \mathbf{I} + \mathbf{B}_{L-1,\sigma}(\tilde{\mathbf{h}}_{L-1}) \mathbf{B}_{L-2,\sigma}(\tilde{\mathbf{h}}_{L-2}) \dots \mathbf{B}_{0,\sigma}(\tilde{\mathbf{h}}_0) = \mathbf{I} + \prod_{l=L-1}^0 \mathbf{B}_{l,\sigma}(\tilde{\mathbf{h}}_l) \quad (3.52)$$

By casting the fermionic trace as a product of determinants, we obtained the computable approximation of the distribution operator \mathcal{P} corresponding to Z_β as advertised in Eq.(1.17).

$$P(\mathbf{h}) = \frac{A}{Z_{\mathbf{h}}} \det[\mathbf{M}_\uparrow(\mathbf{h})] \det[\mathbf{M}_\downarrow(\mathbf{h})], \quad (3.53)$$

where $A = (c_U)^{NL}$ is a normalization constant. This is now a distribution function over configurations of the field \mathbf{h} since the problem is “classical” (the quotes serve to emphasize that $P(\mathbf{h})$ can be negative)!

For the particular case of no interactions $U = 0$, we have that $\nu = 0$, and $\mathbf{M}_\sigma(\mathbf{h})$ are independent of the HS-field. The Trotter-Suzuki approximation then becomes exact and the Hubbard Hamiltonian may be simulated exactly after evaluating $\mathbf{M}_\sigma(\mathbf{h})$ a single time. Monte Carlo sampling is not required.

We mapped a d -dimensional quantum problem to a $(d+1)$ -dimensional “classical” problem with an extra imaginary-time dimension. Note that the size of the state space might have been increased to 2^{NL} (assuming that $L > 2$), and even if it didn’t, it still remains exponential. However, it can now be probed more easily: while we might have increased the number of possible configurations by introducing the mapping, we arrived at a form which is tractable by a standard Monte Carlo method, as described in the previous section. This is because we may now efficiently navigate through the exponentially large state space of the system using importance sampling. Schematically, the degrees of freedom of the quantum problem correspond to the i -indices of the c -operators. In our formulation, an additional imaginary time slice index l was introduced, leading to a mapping that is not specific to the Hubbard model, but applies generally for any quantum system.

3.2.4 Monte Carlo sampling of the HS-field

The computational problem is now that of sampling configurations of the \mathbf{h} field drawn from the distribution $P(\mathbf{h})$ using *Classical* Monte Carlo. It remains to choose a dynamics and a sampling scheme. The simplest strategy to change from a configuration \mathbf{h} to a new one \mathbf{h}' is single spin-flip dynamics. We choose a random point (l, i) , and we flip the spin at that space-time “site”: $h'_{l,i} = -h_{l,i}$, keeping all others unchanged. The most common scheme to ensure that the distribution of the accepted sample is $P(\mathbf{h})$ is the Metropolis-Hastings algorithm, but other choices exist, such as the heat bath algorithm. After the warm-up steps, we are correctly sampling from the required distribution, and we may perform measurements.

Algorithm 3.1 Auxiliary Field Quantum Monte Carlo Sampling Scheme

```

Initialize HS field  $\mathbf{h}$ 
Initialize hoppings  $\mathbf{K}$ 
 $(h_{l,i}) = (\pm 1)_{l=0,i=0}^{L-1,N-1}$ 
 $(l, i) \leftarrow (0, 0)$ 
5: for step = 1 to  $S$  do
    Propose new configuration by flipping a spin
     $h'_{l,i} = -h_{l,i}$ 
    Compute the acceptance ratio  $a_{l,i}$ 
     $\frac{\det[\mathbf{M}_\uparrow(\mathbf{h}')]\det[\mathbf{M}_\downarrow(\mathbf{h}')]}{\det[\mathbf{M}_\uparrow(\mathbf{h})]\det[\mathbf{M}_\downarrow(\mathbf{h})]}$ 
    Metropolis step
    Draw random number  $r \in [0, 1]$ 
10:   if  $r \leq \min(1, a_{l,i})$  then
         $\mathbf{h} = \mathbf{h}'$ 
    else
         $\mathbf{h} = \mathbf{h}$ 
    end if
15:   Next space-time “site”
    if  $i < N - 1$  then
         $l = l, i = i + 1$ 
    else
        if  $l < L - 1$  then
             $l = l + 1, i = 0$ 
        end if
        if  $l = L - 1$  then
             $l = 0, i = 0$ 
        end if
20:   end if
25: end for

```

The acceptance/rejection scheme leads to a rank-one update of the matrices $\mathbf{M}_\sigma(\mathbf{h})$ ⁴, which affords an efficient evaluation of the acceptance ratio $a_{l,i}$ [56] (see appendix B). The acceptance ratio is given in terms of determinants of the Green’s matrices, but these need not be explicitly computed at each step. Instead, a *global* update of the Green’s matrices at each step suffices to obtain the ratio between the determinants of the Green’s matrices of the current and previous configurations. This brings the computational complexity from $\mathcal{O}(N^3)$ to $\mathcal{O}(N^2)$ at each step. This results in an overall cubic scaling of the algorithm, more precisely $\mathcal{O}(\beta N^3)$ (the process is repeated LN times, and $\beta \sim L$).

Suppose we start at the first imaginary-time slice, $l = 0$. Using the result of appendix B, for $i = 0$, the proposal $h'_{00} = -h_{00}$ leads to

$$r_{00} = \left[1 + \alpha_{0,\uparrow}(1 - \mathbf{e}_0^T \mathbf{M}_\uparrow^{-1}(\mathbf{h}) \mathbf{e}_0) \right] \left[1 + \alpha_{0,\downarrow}(1 - \mathbf{e}_0^T \mathbf{M}_\downarrow^{-1}(\mathbf{h}) \mathbf{e}_0) \right] \equiv d_{0,\uparrow} d_{0,\downarrow}, \quad (3.54)$$

where we defined the unit vectors $\mathbf{e}_0, \mathbf{e}_1, \dots, \mathbf{e}_{N-1}$, and the ratios of determinants

$$d_{i,\sigma} = 1 + \alpha_{i,\sigma}(1 - G_{ii}^\sigma) \quad \text{with} \quad \alpha_{i,\sigma} = e^{-2\sigma\nu h_{li}} - 1$$

The most expensive operation is the computation of the $(0, 0)$ entry of $G^\sigma(\mathbf{h})$. However, this object is always computed in advance (it is the main object of the simulation!), so the computation of the acceptance ratio is essentially free. Whenever a step is accepted, the Green’s matrices are updated in $\mathcal{O}(N^2)$ flops, and the acceptance ratio is recomputed as our notation suggests

⁴We will see that it is actually more convenient to work with their inverses, the Green’s matrices.

$$\mathbf{G}^\sigma(\mathbf{h}) \leftarrow \mathbf{G}^\sigma(\mathbf{h}) - \frac{\alpha_{i,\sigma}}{r_{l,i}} \mathbf{u}_{i,\sigma} \mathbf{w}_{i,\sigma}^T \quad r_{l,i} = d_{i,\uparrow} d_{i,\downarrow}, \quad (3.55)$$

where $\mathbf{u}_{i,\sigma} = (\mathbf{I} - \mathbf{G}^\sigma(\mathbf{h}))\mathbf{e}_i$, and $\mathbf{w}_{i,\sigma} = [\mathbf{G}^\sigma(\mathbf{h})]^T \mathbf{e}_i$. Notice that here, \mathbf{G}^σ is the Green's matrix at slice l .

Notice that only one entry of each of the Green's matrices is used at each step for sampling. To improve the efficiency of our implementation, we can compute only the relevant entry that is required for sampling until a sweep of the space lattice is completed, at which point we need to update the entire Green's function (since this final update has complexity $\mathcal{O}(N^3)$, the complexity of the algorithm does not change, although some speed-up is expected). This block high rank update is a “delayed update” in the sense that we avoid unnecessary computations until they are absolutely needed.

This procedure generalizes for all other time slices. First, note that the order of the operators in Eq.(3.50) may be changed by using the cyclic property of the trace. Concomitantly, for example, when we advance to $l = 1$, we may write the \mathbf{M} -matrices by wrapping the equivalent $\widehat{\mathbf{M}}$ matrices:

$$\mathbf{M}_\sigma(\mathbf{h}) = \mathbf{B}_{0,\sigma}^{-1}(\tilde{\mathbf{h}}_0) \widehat{\mathbf{M}}_\sigma(\mathbf{h}) \mathbf{B}_{0,\sigma}(\tilde{\mathbf{h}}_0) \quad \widehat{\mathbf{M}}_\sigma(\mathbf{h}) = \mathbf{I} + \mathbf{B}_{0,\sigma}(\tilde{\mathbf{h}}_0) \mathbf{B}_{L-1,\sigma}(\tilde{\mathbf{h}}_{L-1}) \mathbf{B}_{L-2,\sigma}(\tilde{\mathbf{h}}_{L-2}) \dots \mathbf{B}_{1,\sigma}(\tilde{\mathbf{h}}_1) \quad (3.56)$$

The Metropolis ratio can be computed with $\widehat{\mathbf{M}}$, and the Green's functions are also wrapped :

$$r = \frac{\det[\mathbf{M}_\uparrow(\mathbf{h}')]\det[\mathbf{M}_\downarrow(\mathbf{h}')]}{\det[\mathbf{M}_\uparrow(\mathbf{h})]\det[\mathbf{M}_\downarrow(\mathbf{h})]} = \frac{\det[\widehat{\mathbf{M}}_\uparrow(\mathbf{h}')]\det[\widehat{\mathbf{M}}_\downarrow(\mathbf{h}')]}{\det[\widehat{\mathbf{M}}_\uparrow(\mathbf{h})]\det[\widehat{\mathbf{M}}_\downarrow(\mathbf{h})]} \quad \widehat{\mathbf{G}}^\sigma(\tilde{\mathbf{h}}_0) = \mathbf{B}_{0,\sigma}(\tilde{\mathbf{h}}_0) \mathbf{G}^\sigma(\mathbf{h}) \mathbf{B}_{0,\sigma}^{-1}(\tilde{\mathbf{h}}_0) \quad (3.57)$$

The wrapping trick makes $\mathbf{B}_{1,\sigma}(\tilde{\mathbf{h}}_1)$ appear at the position of the $\widehat{\mathbf{M}}$ -matrix where $\mathbf{B}_{0,\sigma}(\tilde{\mathbf{h}}_0)$ appeared for $l = 0$. Thus, we can use everything that was derived for $l = 0$ with the wrapped Green's functions $\widehat{\mathbf{G}}^\sigma$. This is repeated consecutively as we advance in imaginary-time.

Since the cost of wrapping is $\mathcal{O}(N^3)$, the cost of computing r is essentially that of updating the Green's matrices. Each update requires $2N^2$ elementary operations, so that a sweep through the HS-matrix \mathbf{h} costs $2N^3L$ flops. One must pay attention to the efficiency (by delayed updates), and stability of the updating and wrapping of the Green's matrices. When numerically divergent scales are present, the instability of this scheme must be controlled by computing the Green's functions from scratch periodically. When doing so, the stability of the product of the (potentially large) chain of \mathbf{B} -matrices is ensured by using QR decomposition with partial pivoting, following QUEST's implementation [56].

3.2.5 Checkerboard Breakup

In this section, we focus on the computation of the matrix exponential $\mathbf{B} = e^{t\Delta\tau\mathbf{K}}$. Although the cost of computing it is small, and it is done only once in the initialization phase of the algorithm, if it is done naively, the resulting matrix is dense. This is undesired since it is multiplied repeatedly by other matrices throughout the algorithm, which has a high cost of order $\mathcal{O}(N^3)$. Diagonalizing and exponentiating \mathbf{K} results in a dense matrix of N^2 elements. For uniform hoppings, we can use the

FFT and apply the kinetic energy $e^{\Delta\tau\mathbf{K}}$ in momentum space, in which \mathbf{K} is diagonal. The drawback of this approach is two-fold: first, the system size becomes constrained to powers of 2, so that the FFT can be applied efficiently, and, more importantly, we cannot apply it to nonuniform hoppings (which is precisely the case we are interested in in this work).

A convenient, and sparse approximation of \mathbf{B} in real space is available, and it is obtained simply by applying the Trotter breakup.

3.3 Measurements

In QMC simulations, physical observables are extracted by measuring them directly over the course of the sampling of the configuration space. The single-particle (equal time) Green's Function is useful to obtain quantities such as density and kinetic energy, and is simply the inverse of the \mathbf{M} -matrix that we already compute to obtain the acceptance ratio at each step. At imaginary-time $\tau = \Delta\tau\lambda$:

$$G_{ij}^\sigma(\tau, \tau) = \left\langle c_{i,\sigma} c_{j,\sigma}^\dagger \right\rangle_{\mathbf{h}} = \left((\mathbf{I} + \prod_{l=\lambda-1}^0 \mathbf{B}_{l,\sigma}(\tilde{\mathbf{h}}_l) \prod_{l=L-1}^\lambda \mathbf{B}_{l,\sigma}(\tilde{\mathbf{h}}_l))^{-1} \right)_{ij} \equiv \left((\mathbf{I} + \mathbf{B}_{\mathbf{h}}^\sigma(\tau, 0) \mathbf{B}_{\mathbf{h}}^\sigma(\beta, \tau))^{-1} \right)_{ij} \quad (3.58)$$

The equal time Green's function is a fermion average for a given HS field configuration [86]. For a fixed HS field, the problem becomes a free fermion problem, and one may use Wick's theorem to write down expressions for more complex observables. Eq.(3.58) is easily shown, and the proof offers some insight into how other observables are written in terms of $G_{ij}^\sigma(\tau, \tau)$ through Wick's theorem. In auxiliary field Quantum Monte Carlo (QMC), we wish to compute averages of observables O by sampling \mathbf{h} configurations, and then averaging O for fixed \mathbf{h} (which is computed throughout the simulation) over these. Ignoring spin,

$$\begin{aligned} \langle O \rangle &= \frac{1}{Z} \text{Tr}[e^{-\beta\mathcal{H}} O] = \sum_{\mathbf{h}} P(\mathbf{h}) \langle O \rangle_{\mathbf{h}} + \mathcal{O}(\Delta\tau^2), \text{ where} \\ P(\mathbf{h}) &= \frac{C(\mathbf{h}) \det[\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, 0)]}{\sum_{\mathbf{h}} C(\mathbf{h}) \det[\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, 0)]} \quad \langle O \rangle_{\mathbf{h}} = \frac{\text{Tr}[U_{\mathbf{h}}(\beta, \tau) O U_{\mathbf{h}}(\tau, 0)]}{\text{Tr}[U_{\mathbf{h}}(\beta, 0)]} \end{aligned} \quad (3.59)$$

and $U_{\mathbf{h}}(\tau', \tau)$ is the imaginary-time evolution operator between τ and τ' . Introducing a fictitious coupling η to a one-body operator $O = \mathbf{c}^\dagger \mathbf{A} \mathbf{c}$ that can be taken back to zero later, we obtain

$$\begin{aligned}
\langle O \rangle_{\mathbf{h}} &= \partial_{\eta} \left(\ln \text{Tr} [U_{\mathbf{h}}(\beta, \tau) e^{\eta O} U_{\mathbf{h}}(\tau, 0)] \right) \Big|_{\eta=0} = \partial_{\eta} \left(\ln \det[\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, \tau) e^{\eta \mathbf{A}} \mathbf{B}_{\mathbf{h}}(\tau, 0)] \right) \Big|_{\eta=0} \\
&= \partial_{\eta} \left(\text{Tr} [\ln(\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, \tau) e^{\eta \mathbf{A}} \mathbf{B}_{\mathbf{h}}(\tau, 0))] \right) \Big|_{\eta=0} = \text{Tr} [\mathbf{B}_{\mathbf{h}}(\tau, 0) (\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, 0))^{-1} \mathbf{B}_{\mathbf{h}}(\beta, \tau) \mathbf{A}] \\
&= \text{Tr} \left[(\mathbf{B}^{-1}(\beta, \tau) \mathbf{B}^{-1}(\tau, 0) + \mathbf{I})^{-1} (\mathbf{B}(\tau, 0) \mathbf{B}(\beta, \tau))^{-1} (\mathbf{B}(\tau, 0) \mathbf{B}(\beta, \tau)) \mathbf{A} \right] \\
&= \text{Tr} \left[(\mathbf{I} + \mathbf{B}(\tau, 0) \mathbf{B}(\beta, \tau))^{-1} (\mathbf{I} + \mathbf{B}(\tau, 0) \mathbf{B}(\beta, \tau) - \mathbf{I}) \mathbf{A} \right] \\
&= \text{Tr} \left[\left(\mathbf{I} - (\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\tau, 0) \mathbf{B}_{\mathbf{h}}(\beta, \tau))^{-1} \right) \mathbf{A} \right]
\end{aligned} \tag{3.60}$$

In particular, for the case of the Green's function: $O = c_i c_j^\dagger$, $A_{xy} = \delta_{ij} - \delta_{xj} \delta_{yi}$, leading to Eq.(3.58). A generalization of Eq.(3.60) for higher order derivatives allows us to obtain the connected correlation functions, or cumulants (denoted $\langle\langle \dots \rangle\rangle_{\mathbf{h}}$), revealing a connection with Wick's theorem. Let

$$\langle\langle O_n O_{n-1} \dots O_1 \rangle\rangle_{\mathbf{h}} = \partial_{\eta_n} \partial_{\eta_{n-1}} \dots \partial_{\eta_1} \ln \text{Tr}[U_{\mathbf{h}}(\beta, \tau) e^{\eta_n O_n} e^{\eta_{n-1} O_{n-1}} \dots e^{\eta_1 O_1} U_{\mathbf{h}}(\tau, 0)] \Big|_{\eta_n=\eta_{n-1}=\dots=\eta_1=0} \tag{3.61}$$

we see a pattern emerging, relating multi-point correlators and cumulants. Omitting the subscript \mathbf{h} :

$$\begin{aligned}
\langle\langle O_1 \rangle\rangle &= \langle O_1 \rangle \\
\langle\langle O_2 O_1 \rangle\rangle &= \langle O_2 O_1 \rangle - \langle O_2 \rangle \langle O_1 \rangle \\
\langle\langle O_3 O_2 O_1 \rangle\rangle &= \langle O_3 O_2 O_1 \rangle - \langle O_3 \rangle \langle\langle O_2 O_1 \rangle\rangle - \langle O_2 \rangle \langle\langle O_3 O_1 \rangle\rangle - \langle O_1 \rangle \langle\langle O_3 O_2 \rangle\rangle - \langle O_1 \rangle \langle O_2 \rangle \langle O_3 \rangle \\
\langle O_n O_{n-1} \dots O_1 \rangle &= \langle\langle O_n O_{n-1} \dots O_1 \rangle\rangle + \sum_{j=1}^n \langle\langle O_n \dots \widehat{O}_j \dots O_1 \rangle\rangle \langle\langle O_j \rangle\rangle \\
&\quad + \sum_{j>i} \langle\langle O_n \dots \widehat{O}_j \dots \widehat{O}_i \dots O_1 \rangle\rangle \langle\langle O_j O_i \rangle\rangle + \dots + \langle\langle O_n \rangle\rangle \langle\langle O_{n-1} \rangle\rangle \dots \langle\langle O_1 \rangle\rangle,
\end{aligned} \tag{3.62}$$

where the operators with a hat \widehat{O}_j are excluded from the sum. This is equivalent to the zero temperature version of Wick's theorem that we state in appendix A, Eq.(A.37).

We can now compute the cumulants order by order. In particular, one can show that operators of the type $\langle\langle c_{x_n}^\dagger c_{y_n} c_{x_{n-1}}^\dagger \dots c_{x_1}^\dagger c_{y_1} \rangle\rangle_{\mathbf{h}}$ can always be written in terms of a linear combination of products of pair averages of the type $\langle c^\dagger c \rangle$ [58] A case of particular relevance for the observables we shall be interested in is obtained by doing so for a four c -operator average, i.e. $n = 2$, and $A_{xy}^{(i)} = \delta_{x,x_i} \delta_{y,y_i} \dots$

Before proceeding, recall that, for an invertible matrix \mathbf{A} , the derivative of its inverse with respect to a parameter η can be obtained in terms of the derivative of the matrix itself and its inverse. The sought identity is easy to show by using $\mathbf{A}^{-1} \mathbf{A} = \mathbf{I}$ and differentiating both the LHS and the RHS: $\partial_{\eta}(\mathbf{A}^{-1} \mathbf{A}) = 0 \iff (\partial_{\eta} \mathbf{A}) \mathbf{A}^{-1} + \mathbf{A} \partial_{\eta} \mathbf{A}^{-1} = 0 \iff \partial_{\eta} \mathbf{A}^{-1} = -\mathbf{A}^{-1} (\partial_{\eta} \mathbf{A}) \mathbf{A}^{-1}$.

$$\begin{aligned}
\langle \langle c_{x_2}^\dagger c_{y_2} c_{x_1}^\dagger c_{y_1} \rangle \rangle_{\mathbf{h}} &= \partial_{\eta_2} \partial_{\eta_1} \left(\text{Tr} \left[\ln(\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, \tau) e^{\eta_2 \mathbf{A}_2} e^{\eta_1 \mathbf{A}_1} \mathbf{B}_{\mathbf{h}}(\tau, 0)) \right] \right|_{\eta=0} \\
&= \partial_{\eta_2} \text{Tr} \left[(\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, \tau) e^{\eta_2 \mathbf{A}_2} e^{\eta_1 \mathbf{A}_1} \mathbf{B}_{\mathbf{h}}(\tau, 0))^{-1} \mathbf{B}_{\mathbf{h}}(\beta, \tau) e^{\eta_2 \mathbf{A}_2} e^{\eta_1 \mathbf{A}_1} \mathbf{A}_1 \mathbf{B}(\tau, 0) \right] \Big|_{\eta=0} \\
&= \text{Tr} \left[\mathbf{B}_{\mathbf{h}}(\tau, 0) (\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, \tau) \mathbf{B}_{\mathbf{h}}(\tau, 0))^{-1} \mathbf{B}_{\mathbf{h}}(\beta, \tau) \mathbf{A}_2 \mathbf{A}_1 \right] \\
&\quad - \text{Tr} \left[\mathbf{B}_{\mathbf{h}}(\tau, 0) (\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, \tau) \mathbf{B}_{\mathbf{h}}(\tau, 0))^{-1} \mathbf{B}_{\mathbf{h}}(\beta, \tau) \mathbf{A}_2 \mathbf{B}_{\mathbf{h}}(\tau, 0) (\mathbf{I} + \mathbf{B}_{\mathbf{h}}(\beta, \tau) \mathbf{B}_{\mathbf{h}}(\tau, 0))^{-1} \mathbf{B}_{\mathbf{h}}(\beta, \tau) \mathbf{A}_1 \right] \\
&= \text{Tr}[(\mathbf{I} - \mathbf{G}) \mathbf{A}_2 \mathbf{A}_1] - \text{Tr}[(\mathbf{I} - \mathbf{G}) \mathbf{A}_2 (\mathbf{I} - \mathbf{G}) \mathbf{A}_1] = \text{Tr}[(\mathbf{I} - \mathbf{G}) \mathbf{A}_2 \mathbf{G} \mathbf{A}_1] = \langle c_{x_2}^\dagger c_{y_1} \rangle_{\mathbf{h}} \langle c_{y_2} c_{x_1}^\dagger \rangle_{\mathbf{h}},
\end{aligned} \tag{3.63}$$

where, in the last step, we simply identify the only element of the matrix $(\mathbf{I} - \mathbf{G}) \mathbf{A}_2 \mathbf{G} \mathbf{A}_1$ that is on the diagonal, which is the only one that is picked up by the trace. By comparison with Eq.(3.62), we obtain an important relation we will use repeatedly:

$$\langle c_{x_2}^\dagger c_{y_2} c_{x_1}^\dagger c_{y_1} \rangle_{\mathbf{h}} = \langle c_{x_2}^\dagger c_{y_2} \rangle_{\mathbf{h}} \langle c_{x_1}^\dagger c_{y_1} \rangle_{\mathbf{h}} + \langle c_{x_2}^\dagger c_{y_1} \rangle_{\mathbf{h}} \langle c_{y_2} c_{x_1}^\dagger \rangle_{\mathbf{h}} \tag{3.64}$$

3.3.1 Obtaining observables in terms of Green's functions

The simplest observable that can be obtained from the Green's function is the (site-dependent) electron density

$$\rho_{i,\sigma} = \langle c_{i,\sigma}^\dagger c_{i,\sigma} \rangle = 1 - \langle c_{i,\sigma} c_{i,\sigma}^\dagger \rangle = 1 - G_{ii}^\sigma, \tag{3.65}$$

It is natural to think of averaging it over the lattice, which is justified by the fact that the Hubbard Hamiltonian is translationally invariant. Thus, $\rho_{i,\sigma}$ should be independent of the spatial site. This statement is strict when exactly solving the model, but it becomes only approximate, i.e. valid only on average in our simulations. Thus, we take the average

$$\rho = \frac{1}{N} \sum_{\sigma} \sum_{i=0}^{N-1} \rho_{i,\sigma} = 2 - \frac{1}{N} \sum_{\sigma} \sum_{i=0}^{N-1} G_{ii}^\sigma \tag{3.66}$$

in an attempt to reduce statistical errors.

One must pay attention to the symmetry of the model at hand, since a similar model for a disordered system including randomness would not be translationally invariant anymore. Moreover, it is implicit that $\rho_{i,\sigma}$ is already averaged over the HS-field configurations that were sampled through the simulation.

The average kinetic energy is similarly obtained.

$$\langle \mathcal{H}_K \rangle = -t \sum_{\langle i,j \rangle, \sigma} \langle (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \rangle = t \sum_{\langle i,j \rangle, \sigma} (G_{ij}^\sigma + G_{ji}^\sigma) = t \sum_{i,j,\sigma} K_{ij} (G_{ij}^\sigma + G_{ji}^\sigma), \tag{3.67}$$

where the minus sign is due to the switching of the order of the operators bringing the c^\dagger to the right.

3.3.2 Correlation functions

One of the most important goals of QMC simulations is to inspect the system for order of various types, and to find associated phase transitions. This is done by computing correlation functions $C(j)$, measuring how correlated two sites separated by a distance j are.

$$C(j) = \langle \mathcal{O}_{i+j} \mathcal{O}_i^\dagger \rangle - \langle \mathcal{O}_{i+j} \rangle \langle \mathcal{O}_i^\dagger \rangle, \quad (3.68)$$

where \mathcal{O} is an operator corresponding to the order parameter of the phase transition. For example, we might be looking for magnetic order, in which case the relevant operators are S_i^z , i.e. $\mathcal{O}_i = n_{i\uparrow} - n_{i\downarrow}$, $\mathcal{O}_i^\dagger = n_{i\uparrow} - n_{i\downarrow}$, or superconductivity, where we would like to measure correlations in fermion pair formation: $\mathcal{O}_i = c_{i\downarrow} c_{i\uparrow}$, $\mathcal{O}_i^\dagger = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$.

In general, we expect a high temperature disordered phase, for which correlations decay exponentially $C(j) \propto e^{-j/\xi}$, where ξ is a characteristic length called the correlation length. At some point, there can be a transition to a low temperature phase, where $C(j) \propto m^2$, where m is the order parameter for the transition. Right at the transition, that is at $T = T_c$, there might be singular behavior. In continuous phase transitions, the correlation length diverges $\xi \propto (T - T_c)^{-\nu}$, and the correlations decay slower (in fact algebraically): $C(j) \propto j^{-\eta}$, in an intermediate behavior between exponential decay and a constant. The *critical* exponents ν , and η are characteristic of the transition, or more accurately, of the universality class it belongs to.

The behavior of all these quantities on finite lattices does not precisely correspond to the infinite system behavior. The tails of the functions, i.e. the $j \rightarrow \infty$ limit is not well captured. Finite-size scaling is a method to improve on these predictions.

To evaluate correlation functions we use Wick's theorem. Expectations of more than two fermion creation and annihilation operators reduce to products of expectations of pairs of creation and annihilation operators. For example, for spin order in x/y direction:

$$\langle C(j) \rangle = \langle c_{i+j,\downarrow}^\dagger c_{i+j,\uparrow} c_{i,\uparrow}^\dagger c_{i,\downarrow} \rangle = G_{i+j,i}^\uparrow G_{i,i+j}^\downarrow \quad (3.69)$$

How would one measure a correlation function experimentally? Fortunately, there is a quantity that is easy to measure called structure factor, which is just the Fourier transform of the correlation function

$$S(\mathbf{q}) = \sum_j e^{i\mathbf{q} \cdot \mathbf{R}_j} C(j) \quad (3.70)$$

The accuracy of QMC simulations can be evaluated by comparing the results for the Fourier transformed correlation functions with the corresponding experimentally measured structure factors.

3.4 Stabilization

The Green's function is needed both to perform importance sampling and to make measurements. Naively, its computation would involve multiplying a long chain of \mathbf{B} -matrices, adding the identity,

and then taking the inverse. We saw that this costly procedure can be substituted by a more efficient update scheme, which involves wrapping the Green's function as one sweeps between imaginary time slices.

The stability of this procedure depends on the conditioning of the matrices at hand. As the temperature is lowered, or the system size increased, round-off errors accumulate and precision is gradually lost. Thus, we must compute the Green's function from scratch “naively”.

As β increases more and more, the problem becomes so severe that the Green's function cannot be computed at all! This is an effect due to finite-precision in computers. B -matrices potentially contain largely different energy scales. As more and more of them are multiplied together, the condition number of the product increases, and the situation worsens, with the energy scales becoming exponentially divergent.

4

Applications

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In this chapter, we benchmark and compare our code with other implementations by simulating the Hubbard model in 1D and on the 2D square lattice, for which results are well established from either an analytical or numerical perspective. Then, we consider the honeycomb lattice with both periodic and nanoribbon boundary conditions. Finally, we carry out original calculations, applying our code to a minimal model of TMD nanoribbons. We compare our QMC results with those also obtained by us in the mean field approximation. The latter is formulated allowing a site and orbital-dependent mean field, and the self-consistency relation is solved numerically. We characterize the convergence issues arising in this iterative procedure.

4.1 One-dimensional Chain

The main result of the analytical solution of the 1D Hubbard model is that there is no Mott transition. The system remains an insulator down to $U \rightarrow 0$, and becomes a conductor only at $U = 0$. Thus, we expect antiferromagnetic order to appear for high enough β . We can identify it by studying the spin-spin correlation function, and Fourier transforming to obtain a peak at $q = \pi$ in the magnetic structure factor $S(q)$.

4.2 Square lattice

The case of the square lattice is extensively studied, notably in [57]. Mean field results suggest that antiferromagnetic order persists even at weak coupling.

4.3 Honeycomb lattice

This type of geometry is important because of this model's realization in graphene. Moreover, it is interesting to compare these results with those for nanoribbons, which have different boundary conditions, and, in the case of Transition Metal Dichalcogenides (TMDs), multi-orbital nonuniform hoppings between sites of one of the sublattices (the M -atom sublattice).

4.4 Nanoribbons

In this section, we apply our code to the case of honeycomb lattices with boundary conditions corresponding to nanoribbons. These structures are much longer on one direction than on the other, resembling a ribbon, hence their name. The low energy electronic states on the edges of this ribbon might lead to interesting magnetic behavior in TMD nanostructures (as indeed they do in graphene nanostructures [27]) and it is this possibility was unexplored numerically before this work [44, 45], as was mentioned on chapter 1. A nanoribbon is much longer on one direction than on the other, i.e. $l \gg w$. This condition corresponds to taking $N_x \gg N_y$ in our conventions (see Fig.(4.1), where this condition is, of course, not obeyed solely for the sake of giving a good visual representation of the boundary conditions, and the numbering system).

4.4.1 Graphene

We use three coordinates to label each site on the honeycomb lattice, by taking advantage of its bipartite nature. Regarding the honeycomb lattice as two interpenetrating triangular sublattices \mathcal{A} and \mathcal{B} , we take the axes x and y to be along the primitive vectors of each triangular sublattice. Along the x -direction, the ribbon is supposed to be very long, which justifies the fact that we take Periodic boundary conditions (PBCs). In contrast, in the narrow y -direction we take Open boundary conditions (OBCs). To number the sites on the ribbon, we introduce an additional coordinate labeling the sublattice: $z = 0$, if the site is in sublattice \mathcal{A} , and $z = 1$ if the site is in sublattice \mathcal{B} . We then adopt the numbering convention for the sites $i = 0, 1, \dots, 2N_x N_y - 1$ of the lattice \mathcal{L} :

$$i(x, y, z) = N_x N_y z + N_x y + x, \quad (4.1)$$

where $x = 0, \dots, N_x - 1$, $y = 0, \dots, N_y - 1$, and $z = 0, 1$ define each element $\mathbf{r} = (x, y, z) \in \mathcal{L}$.

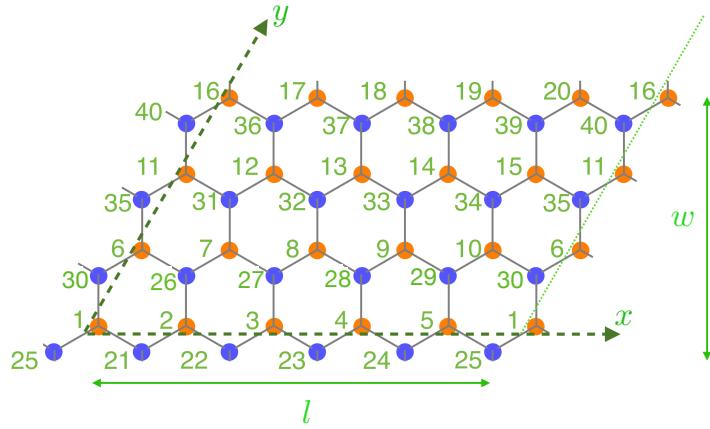


Figure 4.1: Boundary conditions on the nanoribbon for $N_x = 5$, $N_y = 4$. The orange circles correspond to sublattice \mathcal{A} , and the blue circles correspond to sublattice \mathcal{B} . The counting starts at 1 (i.e. the numbers correspond to $i + 1$, since i starts at 0).

The geometry of the system appears through the hopping matrix \mathbf{K} in our code. This numbering system makes it straightforward to find the neighbors of each site. Let us begin by considering a site that is not on a zigzag edge. There are two possible cases. For example, for

$$z_i = 0, y_i \neq N_y - 1, x_i \neq 0,$$

we have that the nearest neighbors of i are $j(i) = \{j(\mathbf{r})\}$, with \mathbf{r} in

$$\left\{ \mathbf{r}_j \in \mathcal{L} \mid z_j = 1 \wedge \left[\left(y_j = y_i \wedge (x_j = x_i \vee x_j = x_i - 1) \right) \vee \left(y_j = y_i + 1 \wedge x_j = x_i - 1 \right) \right] \right\}$$

As opposed to the sites of a honeycomb lattice with PBCs, which have 3 neighbors, the sites of the zigzag edges have only 2 neighbors. We summarize all possible cases in the following table.

Table 4.1: Nearest neighbors on the graphene nanoribbon. The neighbors in red are only for sites that are not on the edges.

OBCs (PBCs)				
Case	z_j	y_j	x_j	
$z_i = 0$	1	y_i	x_i	
			$N_x - 1 - (N_x - x_i) \% N_x$	
$z_i = 1$	0	y_i	x_i	
			$(x_i + 1) \% N_x$	
		$y_i + 1$	$y_i - 1$	

4.4.2 TMDs

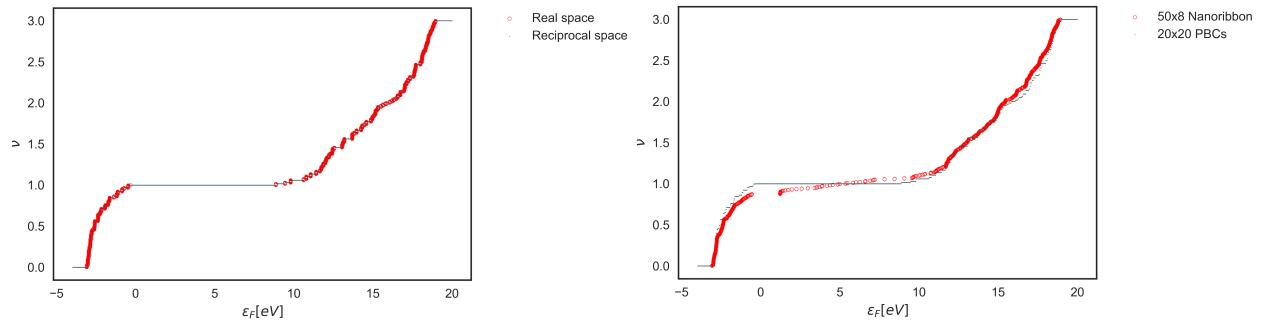


Figure 4.2: Left: Filling factor as a function of the Fermi energy for a system with PBCs, as computed by diagonalizing the input matrix of our code, and by the hopping matrix in k -space. Right: Comparison between the filling factors of a nanoribbon and a periodic system as a function of the Fermi energy, as computed by diagonalizing our input matrix.

5

Conclusions and Future Work

Conclusions Chapter

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A

Obtaining and Solving the Hubbard
Model Approximately and in Simple
Limits

A.1 Hartree-Fock Approximation and the Self Consistent Field Method

In the mean field approximation, the quartic term of the interaction part of the Hamiltonian

$$V_{\text{int}} = \frac{1}{2} V_{\nu' \mu'}^{\nu \mu} c_{\nu}^{\dagger} c_{\mu}^{\dagger} c_{\mu'} c_{\nu'},$$

becomes a sum of all possible 2-body terms (note that terms of the type $\langle cc \rangle$ and $\langle c^{\dagger}c^{\dagger} \rangle$ must vanish since they do not conserve the number of particles).

$$c_{\nu}^{\dagger} c_{\mu}^{\dagger} c_{\mu'} c_{\nu'} \approx -\langle c_{\nu}^{\dagger} c_{\mu'} \rangle c_{\mu}^{\dagger} c_{\nu'} - \langle c_{\mu}^{\dagger} c_{\nu'} \rangle c_{\nu}^{\dagger} c_{\mu'} + \langle c_{\nu}^{\dagger} c_{\nu'} \rangle c_{\mu}^{\dagger} c_{\mu'} + \langle c_{\mu}^{\dagger} c_{\mu'} \rangle c_{\nu}^{\dagger} c_{\nu'}, \quad (\text{A.1})$$

where we ignored the constant terms which are unimportant in the Hamiltonian, in what concerns the dynamics.

This Hartree-Fock, or mean field approximation is slightly tricky to obtain. It requires one to be precise about what the meaning of the mean field approximation is in terms of creation and annihilation operators. In mean field theory, we assume that the operator

$$\rho_{\mu \mu'} = c_{\mu}^{\dagger} c_{\mu'} \quad (\text{A.2})$$

is close to its average, so that we neglect second order terms in the fluctuations $\delta \rho_{\mu \mu'}$, i.e. $\rho_{\mu \mu'}$ is “large” only when its average is nonzero, otherwise it is negligibly small. Thus, for most combinations of indices, this operator will vanish. We follow the usual mean field procedure of writing the original operator as a deviation plus an average

$$c_{\nu}^{\dagger} \left(c_{\mu}^{\dagger} c_{\mu'} - \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \right) c_{\nu'} + c_{\nu}^{\dagger} c_{\nu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle \quad (\text{A.3})$$

Then we note that if $\nu' \neq \mu$, we can commute $c_{\nu'}$ with the parenthesis. But this is true except in a set of measure zero. In the thermodynamic limit $N \rightarrow \infty$, the number of allowed \mathbf{k} -states is very large, and if we take a continuum limit in which the set of possible \mathbf{k} -states becomes dense, then the commutation becomes exact. Repeating the procedure of writing (A.3) replacing $c_{\nu}^{\dagger} c_{\nu'} \mapsto c_{\nu}^{\dagger} c_{\nu'} - \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + \langle c_{\nu}^{\dagger} c_{\nu'} \rangle$, we obtain

$$\underbrace{(c_{\nu}^{\dagger} c_{\nu'} - \langle c_{\nu}^{\dagger} c_{\nu'} \rangle)(c_{\mu}^{\dagger} c_{\mu'} - \langle c_{\mu}^{\dagger} c_{\mu'} \rangle)}_{\propto \delta \rho_{\mu \mu'} \delta \rho_{\nu \nu'}} + c_{\nu}^{\dagger} c_{\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle + c_{\mu}^{\dagger} c_{\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle - \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle \quad (\text{A.4})$$

But this result is not complete. This is only the so called Hartree or direct term. Due to identical nature of the interacting electrons, we must consider an analogous contribution for $\langle c_{\nu}^{\dagger} c_{\mu'} \rangle$ finite. We start by exchanging the first two operators:

$$c_{\nu}^{\dagger} c_{\mu}^{\dagger} c_{\mu'} c_{\nu'} = -c_{\mu}^{\dagger} c_{\nu}^{\dagger} c_{\mu'} c_{\nu'} \quad (\text{A.5})$$

Then we proceed in exactly the same manner as before. The result is analogous, but a minus sign appears and we must switch $\mu \leftrightarrow \nu$:

$$-c_\mu^\dagger c_{\nu'} \langle c_\nu^\dagger c_{\mu'} \rangle - c_\nu^\dagger c_{\mu'} \langle c_\mu^\dagger c_{\nu'} \rangle + \langle c_\nu^\dagger c_{\mu'} \rangle \langle c_\mu^\dagger c_{\nu'} \rangle \quad (\text{A.6})$$

Ignoring the constant terms of the type $\langle c^\dagger c \rangle \langle c^\dagger c \rangle$, we recover equation (A.1).

Now we can simply substitute the mean field expansion of equation (A.1) in the second term to obtain the last term that is subtracted in equation (2.1) (we omit the boldface on the \mathbf{k} 's solely in the following equation, but keep in mind that they are vectors):

$$\begin{aligned} & \frac{1}{2} \sum_{\substack{k_1 k_2 k'_1 k'_2 \\ \sigma_1 \sigma_2}} V_{k'_1 k'_2}^{k_1 k_2} \left(-\underbrace{\left\langle c_{k_1 \sigma_1}^\dagger c_{k'_2 \sigma_2} \right\rangle}_{\delta_{k_1 k'_2} \delta_{\sigma_1 \sigma_2} f_{k_1}} c_{k_2 \sigma_2}^\dagger c_{k'_1 \sigma_1} - \underbrace{\left\langle c_{k_2 \sigma_2}^\dagger c_{k'_1 \sigma_1} \right\rangle}_{\delta_{k_2 k'_1} \delta_{\sigma_1 \sigma_2} f_{k_2}} c_{k_1 \sigma_1}^\dagger c_{k'_2 \sigma_2} + \underbrace{\left\langle c_{k_1 \sigma_1}^\dagger c_{k'_1 \sigma_1} \right\rangle}_{\delta_{k_1 k'_1} f_{k_1}} c_{k_2 \sigma_2}^\dagger c_{k'_2 \sigma_2} \right. \\ & \left. + \underbrace{\left\langle c_{k_2 \sigma_2}^\dagger c_{k'_2 \sigma_2} \right\rangle}_{\delta_{k_2 k'_2} f_{k_2}} c_{k_1 \sigma_1}^\dagger c_{k'_1 \sigma_1} \right) \end{aligned} \quad (\text{A.7})$$

In the language of Hartree Fock theory, the first two terms give the exchange term, and the last two terms the direct term. Apart from the $\frac{1}{2}$ factor, the term in (A.7) becomes

$$\begin{aligned} & - \sum_{\substack{k_1 k_2 \\ k'_1 \sigma_1}} V_{k'_1 k_1}^{k_1 k_2} f_{k_1} c_{k_2 \sigma_1}^\dagger c_{k'_1 \sigma_1} - \sum_{\substack{k_1 k_2 \\ k'_2 \sigma_1}} V_{k_2 k'_2}^{k_1 k_2} f_{k_2} c_{k_1 \sigma_1}^\dagger c_{k'_2 \sigma_1} + \sum_{\substack{k_1 k_2 k'_2 \\ \sigma_1 \sigma_2}} V_{k_1 k'_2}^{k_1 k_2} f_{k_1} c_{k_2 \sigma_2}^\dagger c_{k'_2 \sigma_2} \\ & + \sum_{\substack{k_1 k_2 k'_1 \\ \sigma_1 \sigma_2}} V_{k'_1 k'_2}^{k_1 k_2} f_{k_2} c_{k_1 \sigma_1}^\dagger c_{k'_1 \sigma_1} \\ & = \sum_{k_1 k_2 \sigma_1} \left(4V_{k_1 k_2}^{k_1 k_2} - 2V_{k_2 k_1}^{k_1 k_2} \right) f_{k_2} c_{k_1 \sigma_1}^\dagger c_{k_1 \sigma_1}, \end{aligned} \quad (\text{A.8})$$

where we used momentum conservation to eliminate a k' -sum. Moreover, we used that the sum on spin ($\pm 1/2$) on the last two terms gives factors of 2, since the interaction is spin independent and thus no spin-dependent term remains after we use momentum conservation. Making $k_1 \rightarrow k$, $k_2 \rightarrow k'$, $\sigma_1 \rightarrow \sigma$, and recalling the definition in equation (2.2), we obtain the result we sought.

The procedure above is meant to serve as an intuitive derivation. Now we approach the problem more formally. In fact, the argument that allowed us to perform the commutation leading to equation A.4 seems somewhat handwaving. We should not have to take the thermodynamic limit to perform a mean field expansion. A more systematic procedure to obtain the mean field expansion of a quartic interaction term was given by Pierre de Gennes in the context of a mean field treatment of a superconductor in a magnetic field [87]. Our case is actually much simpler to analyze, but we follow the same argument as de Gennes.

Consider the Hamiltonian to be given by $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where

$$\begin{aligned}\mathcal{H}_0 &= \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \\ \mathcal{H}_1 &= \frac{1}{2} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \mathbf{k}'_1 \mathbf{k}'_2 \\ \sigma_1 \sigma_2}} V_{\mathbf{k}_1 \mathbf{k}_2}^{k_1 k_2} c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_2 \sigma_2} c_{\mathbf{k}'_1 \sigma_1}\end{aligned}\tag{A.9}$$

We would like to find an effective Hamiltonian that is quadratic in the fermion operators:

$$\mathcal{H}_{\text{eff}} = \sum_{\mathbf{k}, \sigma} (\varepsilon_{\mathbf{k}} + v_{\mathbf{k}}) c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma}\tag{A.10}$$

This effective Hamiltonian is diagonal, so assuming we know $v_{\mathbf{k}}$ (which is what we are trying to determine in the first place), we can compute its eigenstates $\{|\phi\rangle\}$, and compute the average of the actual Hamiltonian \mathcal{H} using the basis $\{|\phi\rangle\}$:

$$\langle \mathcal{H} \rangle = \frac{\sum_{\phi} \langle \phi | \mathcal{H} | \phi \rangle e^{-\beta E_{\phi}}}{\sum_{\phi} e^{-\beta E_{\phi}}}\tag{A.11}$$

Our criterion to determine \mathcal{H}_{eff} is the requirement that the free energy $F = \langle \mathcal{H} \rangle - TS$, with the average computed with the eigenstates of \mathcal{H}_{eff} be stationary, i.e. $\delta F = 0$. Thus, we find the mean field form of the quartic term invoking only a variational principle without any need to resort to the thermodynamic limit. In fact, we never even have to explicitly compute the average in equation (A.11). In terms of pairs of fermion operator averages, we have

$$\langle \mathcal{H} \rangle = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} \left\langle c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \right\rangle + \frac{1}{2} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \mathbf{k}'_1 \mathbf{k}'_2 \\ \sigma_1 \sigma_2}} V_{\mathbf{k}_1 \mathbf{k}_2}^{k_1 k_2} \left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_2 \sigma_2} c_{\mathbf{k}'_1 \sigma_1} \right\rangle,\tag{A.12}$$

where the last term can be reduced to products of averages of pairs of fermion operators by Wick's theorem:

$$\begin{aligned}\left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_2 \sigma_2} c_{\mathbf{k}'_1 \sigma_1} \right\rangle &= \left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}'_1 \sigma_1} \right\rangle \left\langle c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_2 \sigma_2} \right\rangle - \left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}'_2 \sigma_2} \right\rangle \left\langle c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_1 \sigma_1} \right\rangle \\ &+ \left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}_2 \sigma_2}^\dagger \right\rangle \left\langle c_{\mathbf{k}'_2 \sigma_2} c_{\mathbf{k}'_1 \sigma_1} \right\rangle\end{aligned}\tag{A.13}$$

The computation is now done by using the rules (for all \mathbf{k} and σ).

$$\begin{aligned}\left\langle c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}', \sigma'} \right\rangle &= \delta_{\mathbf{k}, \mathbf{k}'} \delta_{\sigma, \sigma'} f_{\mathbf{k}} \\ \left\langle c_{\mathbf{k}, \sigma}^{(\dagger)} c_{\mathbf{k}', \sigma'}^{(\dagger)} \right\rangle &= 0,\end{aligned}\tag{A.14}$$

where $f_{\mathbf{k}} = (e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} + 1)^{-1}$ is the Fermi-Dirac function.

Since the original Hamiltonian is quadratic, again we have that terms of the type $\langle cc \rangle$ and $\langle c^\dagger c^\dagger \rangle$ do not contribute. Hence, varying the free energy, we obtain

$$\delta F = \delta \langle \mathcal{H} \rangle - T\delta S = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \delta \left\langle c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \right\rangle + \frac{1}{2} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \mathbf{k}'_1 \mathbf{k}'_2 \\ \sigma_1 \sigma_2}} V_{\mathbf{k}'_1 \mathbf{k}'_2}^{k_1 k_2} \left(\left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}'_1 \sigma_1} \right\rangle \delta \left\langle c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_2 \sigma_2} \right\rangle + \right. \\ \left. \delta \left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}'_1 \sigma_1} \right\rangle \left\langle c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_2 \sigma_2} \right\rangle - \left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}'_2 \sigma_2} \right\rangle \delta \left\langle c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_1 \sigma_1} \right\rangle - \delta \left\langle c_{\mathbf{k}_1 \sigma_1}^\dagger c_{\mathbf{k}'_2 \sigma_2} \right\rangle \left\langle c_{\mathbf{k}_2 \sigma_2}^\dagger c_{\mathbf{k}'_1 \sigma_1} \right\rangle \right) - T\delta S, \quad (\text{A.15})$$

which can be simplified exactly in the same manner as in equation (A.7), i.e. by using the rules of equation (A.14), and that the occupation of a given momentum state \mathbf{k} is given by the Fermi-Dirac function:

$$\delta F = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \delta \left\langle c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \right\rangle + \sum_{\mathbf{k}\mathbf{k}'\sigma} \left(2V_{\mathbf{k}\mathbf{k}'}^{\mathbf{k}\mathbf{k}'} - V_{\mathbf{k}'\mathbf{k}'}^{\mathbf{k}\mathbf{k}'} \right) f_{\mathbf{k}'} c_{\mathbf{k}\sigma} \delta \left\langle c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \right\rangle \quad (\text{A.16})$$

We can now compare $\delta F = \delta \langle \mathcal{H} \rangle - T\delta S$ and $\delta F' = \delta \langle \mathcal{H}_{\text{eff}} \rangle - T\delta S$, which is simply given by

$$\delta F' = \delta \langle \mathcal{H}_{\text{eff}} \rangle - T\delta S = \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} + v_{\mathbf{k}}) \delta \left\langle c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \right\rangle \quad (\text{A.17})$$

Requiring both free energies to be stationary, we find our desired result

$$v_{\mathbf{k}} = \sum_{\mathbf{k}'} \left(2V_{\mathbf{k}\mathbf{k}'}^{\mathbf{k}\mathbf{k}'} - V_{\mathbf{k}'\mathbf{k}'}^{\mathbf{k}\mathbf{k}'} \right) f_{\mathbf{k}'}, \quad (\text{A.18})$$

which agrees with the result obtained from our initial more intuitive, but somewhat less rigorous argument.

A.2 Mott insulators

Band theory was found to be flawed soon after it was introduced. The picture it proposes is simple and generally works pretty well. It is based on considering the electrons to be independently moving under the constant background potential created by the ions. The solutions of the Schrödinger for free electrons in a periodic potential $U(\mathbf{r})$, such that $U(\mathbf{r}) = U(\mathbf{r} + \mathbf{R})$,

$$\left[-\frac{1}{2m} \nabla^2 + U(\mathbf{r}) \right] \psi(\mathbf{r}) = \varepsilon \psi(\mathbf{r}) \quad (\text{A.19})$$

are given by Bloch's theorem: $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$. Note that we made $\hbar = 1$. Replacing this wave function in equation (A.19), we obtain a differential equation for $u_{\mathbf{k}}(\mathbf{r})$, which has in general an infinite number of solutions. We label them with an index n , which we call the band index. To each solution there corresponds a function $\varepsilon_{n\mathbf{k}}$. The set of these functions is known as the band structure. Since electrons are taken to be independent in band theory, the N-electron eigenstates are obtained by placing an electron in each quantum state. Each state is labelled by its energy $\varepsilon_{n\mathbf{k}\sigma}$. Since our model Hamiltonian does not couple spins (via an electron interaction, for example) and assuming there is no external magnetic field and that the system has an inversion center, we have $\varepsilon_{n\mathbf{k}\uparrow} = \varepsilon_{n\mathbf{k}\downarrow}$. In general

there might be energies for which there is no corresponding $\varepsilon_{n\mathbf{k}\sigma}$. These form intervals called forbidden bands¹. Thus, the ground state of our model may be obtained by filling the energy levels starting from the lowest energy state. Two cases are particularly relevant:

- Every band is either fully occupied or empty. The first excited state differs from the ground state by Δ , the separation between the last fully occupied band and the first empty band. It is then impossible to induce the motion of the electrons by applying an arbitrarily small voltage. This is what it means to be an *insulator*. Since there $2N$ states per band, this is not possible unless the number of electrons per unit cell is an even integer.
- One or more of the bands are partially filled. The energy of occupied state of higher energy is named the Fermi energy ε_F . In this case, the separation between the ground state and the first excited state tends to 0 in the thermodynamic limit, $N \rightarrow \infty$. The system may then respond to infinitesimal excitations, which is the definition of a metal.

Band theory made it possible to predict whether a solid would be a metal or an insulator. However, its success rests crucially on the independent electron approximation. Thus, it is not surprising that for compounds with strongly correlated electrons the theory might fail [79]. The Coulomb interaction is in general non negligible, and the effects it leads to are not captured by a mean field approach. One must resort to many-body theory. An example of a many-body effect that band theory doesn't capture is superconductivity. However, this does not deem band theory useless. In fact, the superconducting phase arises due to an instability of a state that is itself well described by band theory [87]. A far greater failure of band theory is that predicts certain compounds with an odd number of electrons per unit cell, such as NiO and La₂CuO₄, to be metals, while in fact they turn out to be (Mott) insulators. Mott devised a simple argument to justify this failure. It is based on considering the elementary electronic excitations of a solid composed by hydrogen atoms as a function of the distance between atoms.

Consider a hypothetical solid consisting of a square lattice with hydrogen atoms on its points. Each unit cell has one hydrogen atom, and consequently one electron. Band theory would predict such a solid to be a metal. However, if the lattice parameter a is large enough, the solid cannot remain a metal. There must be some value of the lattice parameter $a = a_c$ for which the system becomes an insulator. When current flows through a sample of this solid, electrons hop consecutively, reaching positions that can be quite far on the lattice. For a metal, this process occurs even when exciting the system with an infinitesimal amount of energy. How much energy do we need to provide for this process to occur?

If a is large, we have essentially one electron per site at the start. When an electron is displaced, we end up with a hole and a doubly occupied site. The potential energy of such a state is

$$E_{H^-} + E_{H^+} - 2E_H \quad (\text{A.20})$$

Due to the Coulomb repulsion between the two electrons in H^- , this quantity is strictly positive.

¹We disregard surface states that may have energies that fall in the forbidden bands of band theory.

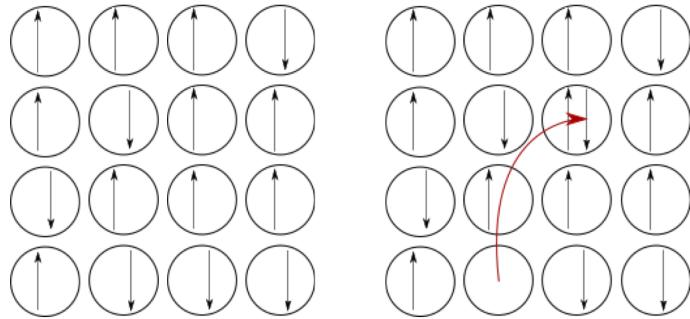


Figure A.1: On the right, a configuration of hydrogen atoms on a square lattice with a hole and a doubly occupied site obtained by delocalization of the spin down electron on the left.

Call it $U > 0$. On the other hand, the system also has kinetic energy: both the hole and the doubly occupied site can delocalize. Let W be the bandwidth corresponding to the delocalization of an electron on the lattice. Both the hole and the doubly occupied will stay at the bottom of the band and gain an energy $W/2$ (assuming that this delocalization is of the same order of magnitude). The dominant transfer integral $-t$ is between nearest neighbors. The dispersion relation then reads

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) \quad (\text{A.21})$$

The bandwidth is then $W = 8t$. The energy of a configuration with a hole and a doubly occupied site is

$$\Delta_c = U - W, \quad (\text{A.22})$$

where U is practically independent of the lattice parameter a . The bandwidth W , however, depends strongly on a . When $a \gg a_0$, where a_0 is the Bohr radius, the transfer integral is exponentially small, because only the exponential tails of the wave functions are relevant. In this limit, $\Delta_c \approx U$ is a large, positive number, and the system is an insulator. This type of insulator is called a Mott insulator, and Δ_c is called the charge gap. As a decreases, t increases, and there must be a critical value $a_c \sim a_0$, for which $U = W$. Below this value, the computation of Δ_c is not valid anymore because the gap cannot be negative. Thus, there must be a metal-insulator transition. It is possible to see this transition if we apply enough pressure to a Mott insulator so as to decrease a and increase t . A transition of this type was first seen in the 1970's for V_2O_3 ². There is a fundamental difference between a band insulator and a Mott insulator. While we must pay an energy Δ_c to make a charge excitation, there is no cost for making a spin excitation: we can flip the spin of an electron without creating a doubly occupied site. The fluctuations of both charge and spin due to the electron interactions may then lead to magnetic behavior characteristic of correlated systems.

²Of course, the transition is not so easy to describe. We should consider the Hubbard model! However, this simple argument provides an intuitive picture.

A.3 Computing the partition function for a quadratic Hamiltonian

Let us start by restating the result we want to prove.

If $\mathcal{H} = \mathbf{c}^\dagger \mathbf{H} \mathbf{c}$, where \mathbf{H} is a $N \times N$ Hermitian matrix, then we have that

$$\text{Tr}[e^{-\beta \mathcal{H}}] = \prod_{i=1}^N (1 + e^{-\beta \lambda_i}), \quad (\text{A.23})$$

where λ_i are the eigenvalues of \mathbf{H} .

We will now prove equation (A.23). Without loss of generality, let us consider \mathbf{H} to be diagonal. Then, its eigenvalues coincide with the diagonal entries, so that $\mathbf{H} = \text{diag}(\lambda_i)$. The quadratic Hamiltonian may then be diagonalized

$$\mathcal{H} = \mathbf{c}^\dagger \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_N) \mathbf{c} = \sum_{i=1}^N \lambda_i n_i$$

We continue by induction. When $N = 1$, we have

$$\text{Tr}(e^{-\beta \mathcal{H}}) = \langle 0 | e^{-\beta \lambda_1 n_1} | 0 \rangle + \langle 1 | e^{-\beta \lambda_1 n_1} | 1 \rangle = 1 + e^{-\beta \lambda_1} \quad (\text{A.24})$$

Assuming that for $N - 1$:

$$\text{Tr}[e^{-\beta \sum_{i=1}^{N-1} \lambda_i n_i}] = \prod_{i=1}^{N-1} (1 + e^{-\beta \lambda_i})$$

we can compute the trace for i going up to N .

$$\begin{aligned} \text{Tr}[e^{-\beta \sum_{i=1}^N \lambda_i n_i}] &= \sum_{i=1}^N \left\langle \psi_1^{\lambda_1} \psi_2^{\lambda_2} \dots \psi_N^{\lambda_N} \middle| e^{-\beta \sum_{i=1}^N \lambda_i n_i} \middle| \psi_1^{\lambda_1} \psi_2^{\lambda_2} \dots \psi_N^{\lambda_N} \right\rangle \\ &= \sum_{i=1}^{N-1} \left(\left\langle \{\psi_i^{\lambda_i}\} 0 \middle| e^{-\beta \sum_{i=1}^N \lambda_i n_i} e^{-\beta \lambda_N n_N} \middle| \{\psi_i^{\lambda_i}\} 0 \right\rangle + \left\langle \{\psi_i^{\lambda_i}\} 1 \middle| e^{-\beta \sum_{i=1}^N \lambda_i n_i} e^{-\beta \lambda_N n_N} \middle| \{\psi_i^{\lambda_i}\} 1 \right\rangle \right) \\ &= (1 + e^{-\beta \lambda_N}) \sum_{i=1}^{N-1} \left\langle \{\psi_i^{\lambda_i}\} \middle| e^{-\beta \lambda_i n_i} \middle| \{\psi_i^{\lambda_i}\} \right\rangle \\ &= (1 + e^{-\beta \lambda_N}) \prod_{i=1}^{N-1} (1 + e^{-\beta \lambda_i}) \\ &= \prod_{i=1}^N (1 + e^{-\beta \lambda_i}) \end{aligned}$$

To complete the proof we note that for any \mathbf{H} , there exists a unitary matrix \mathbf{Q} , such that $\mathbf{Q}^T \mathbf{H} \mathbf{Q} = \mathbf{\Lambda} = \text{diag}(\lambda_i)$. Let $\tilde{\mathbf{c}} = \mathbf{Q} \mathbf{c}$, and $\tilde{n}_i = \tilde{c}_i^\dagger \tilde{c}_i$. Then, we find

$$\mathcal{H} = \mathbf{c}^\dagger \mathbf{H} \mathbf{c} = \tilde{\mathbf{c}}^\dagger \mathbf{\Lambda} \tilde{\mathbf{c}} = \sum_{i=1}^N \lambda_i \tilde{n}_i$$

The trace is independent of the choice of basis functions. Thus, we have

$$\begin{aligned}\text{Tr}(e^{-\beta \mathcal{H}}) &= \text{Tr}\left(\prod_{i=1}^N e^{-\beta \lambda_i \tilde{n}_i}\right) \\ &= \prod_{i=1}^N \left(1 + e^{-\beta \lambda_i}\right) \quad \square\end{aligned}$$

A.4 Density of states for a 1D tight binding model

Using the definition of the density of states

$$N(E) = \frac{1}{N} \sum_{\mathbf{k}} \delta_{E, \varepsilon_{\mathbf{k}}} \rightarrow \frac{1}{(2\pi)^d} \int d\mathbf{k} \delta(E - \varepsilon_{\mathbf{k}}) \text{ when } N \rightarrow \infty. \quad (\text{A.25})$$

with $\varepsilon_k = -2t \cos k$, in the thermodynamic limit we obtain

$$N(E) = \frac{1}{2\pi} \int dk \delta(E + 2t \cos k) \quad (\text{A.26})$$

Now we use a well known property of the delta function

$$\delta(g(x)) = \sum_{\{i|g(x_i)=0\}} \frac{\delta(x - x_i)}{|g'(x_i)|} \quad (\text{A.27})$$

Noting that $g'(k) = -2t \sin k$, and that the roots of g (there are two in the first Brillouin zone, to which the integral is restricted) satisfy $\cos k_i = -E/2t$, so that $\sin k_i = \pm\sqrt{1 - E^2/4t^2}$, we obtain

$$\delta(E + 2t \cos k) = \frac{1}{\sqrt{4t^2 - E^2}} \left(\delta(k - k_1) + \delta(k - k_2) \right) \quad (\text{A.28})$$

leading to the sought result

$$N(E)_{1d} = \frac{1}{\pi\sqrt{4t^2 - E^2}} \quad (\text{A.29})$$

A.5 Obtaining an effective Heisenberg Hamiltonian as the atomic, $U/t \gg 1$ limit of the Hubbard model

To obtain the effective Hamiltonian corresponding to the $U/t \gg 1$ limit of the Hubbard model to second order in degenerate perturbation theory, we start with its general form, as obtained in equation (2.65).

$$\mathcal{H}_{\text{eff}} = -\mathcal{H}_0 \frac{\sum_j n_{j,\sigma} n_{j,-\sigma}}{U} \mathcal{H}_0 \quad (\text{A.30})$$

For each element j of the sum, only terms of the type

$$\sum_{i(j)} c_{j,\sigma}^\dagger c_{i,\sigma}$$

contribute. Here $\sum_{i(j)}$ is a sum over the set of neighbors i of site j .

A term of the effective Hamiltonian \mathcal{H}_{eff} corresponding to the j -th element in the sum reads

$$-\frac{t^2}{U} \sum_{i(j), \sigma_1, \sigma_2} c_{i, \sigma_1}^\dagger c_{j, \sigma_1} n_{j, \sigma} n_{j, -\sigma} c_{j, \sigma_2}^\dagger c_{i, \sigma_2}$$

There are only four cases in which the contribution of a term of this type is nonzero.

- $\sigma = \sigma_1 = \sigma_2$

The operator in the sum then becomes

$$c_{i, \sigma}^\dagger c_{j, \sigma} n_{j, \sigma} n_{j, -\sigma} c_{j, \sigma}^\dagger c_{i, \sigma} = n_{i, \sigma} n_{j, -\sigma} c_{j, \sigma} n_{j, \sigma} c_{j, \sigma}^\dagger$$

Now, we use a fermionic operator identity:

$$\begin{aligned} cn &= cc^\dagger c = (1 - c^\dagger c)c = c \\ \implies c_{j, \sigma} n_{j, \sigma} c_{j, \sigma}^\dagger &= c_{j, \sigma} c_{j, \sigma}^\dagger = 1 - n_{j, \sigma} \end{aligned}$$

The term of the Hamiltonian corresponding to this first case then takes on the form

$$n_{i, \sigma} n_{j, -\sigma} (1 - n_{j, \sigma})$$

We can further simplify this term by noting that in the subspace where \mathcal{H}_{eff} acts, every site is occupied by only a single electron so that

$$n_{j, \sigma} + n_{j, -\sigma} = 1 \iff 1 - n_{j, \sigma} = n_{j, -\sigma}$$

Since, for fermions we have that $\hat{n} = \hat{n}^k$, whichever the power $k \in \mathbb{N}$, the final form of the sought term of the Hamiltonian is

$$n_{i, \sigma} n_{j, -\sigma}$$

- $-\sigma = \sigma_1 = \sigma_2$

The contribution to the Hamiltonian is exactly of the same form but making $\sigma \mapsto -\sigma$:

$$n_{i, -\sigma} n_{j, \sigma}$$

- $\sigma = -\sigma_1 = \sigma_2$

We can use the same reasoning as we did for the first term to obtain

$$\begin{aligned}
& c_{i,-\sigma}^\dagger c_{j,-\sigma} n_{j,\sigma} n_{j,-\sigma} c_{j,\sigma}^\dagger c_{i,\sigma} \\
&= c_{i,-\sigma}^\dagger c_{i,\sigma} \underbrace{c_{j,-\sigma} n_{j,-\sigma}}_{c_{j,-\sigma}} \underbrace{n_{j,\sigma} c_{j,\sigma}^\dagger}_{c_{j,\sigma}^\dagger} \\
&= - c_{i,-\sigma}^\dagger c_{i,\sigma} c_{j,\sigma}^\dagger c_{j,-\sigma}
\end{aligned}$$

- $-\sigma = -\sigma_1 = \sigma_2$

Analogously, the contribution to the Hamiltonian is

$$\begin{aligned}
& c_{i,\sigma}^\dagger c_{j,\sigma} n_{j,\sigma} n_{j,-\sigma} c_{j,-\sigma}^\dagger c_{i,-\sigma} \\
&= - c_{i,-\sigma}^\dagger c_{i,\sigma} c_{j,\sigma}^\dagger c_{j,-\sigma}
\end{aligned}$$

Grouping all these four terms, we obtain

$$\mathcal{H}_{\text{eff}} = \frac{2t^2}{U} \sum_{\langle i,j \rangle} (-n_{i,\sigma} n_{j,-\sigma} + c_{i,-\sigma}^\dagger c_{i,\sigma} c_{j,\sigma}^\dagger c_{j,-\sigma}), \quad (\text{A.31})$$

where the factor of 2 appears because for each pair of nearest neighbors $\langle i,j \rangle$, a term comes from the term $n_{j,\sigma} n_{j,-\sigma}$ of the sum $\sum_j n_{j,\sigma} n_{j,-\sigma}$, and another term from $n_{i,\sigma} n_{i,-\sigma}$.

Recall the second quantized form of the spin operators:

$$\begin{cases} S_i^z = \frac{1}{2}(n_{i,\uparrow} - n_{i,\downarrow}) \\ S_i^+ = c_{i,\uparrow}^\dagger c_{i,\downarrow} \\ S_i^- = c_{i,\downarrow}^\dagger c_{i,\uparrow}, \end{cases} \quad (\text{A.32})$$

Using these relations and that the density operator is $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, the following relations hold

$$\begin{aligned}
S_i^z S_j^z - \frac{1}{4} n_i n_j &= -\frac{1}{2} (n_{i,\uparrow} n_{j,\downarrow} + n_{i,\downarrow} n_{j,\uparrow}) \\
S_i^+ S_j^- + S_i^- S_j^+ &= c_{i,\uparrow}^\dagger c_{i,\downarrow} c_{j,\downarrow}^\dagger c_{j,\uparrow} + c_{i,\downarrow}^\dagger c_{i,\uparrow} c_{j,\uparrow}^\dagger c_{j,\downarrow}
\end{aligned} \quad (\text{A.33})$$

Thus, we may rewrite the effective Hamiltonian:

$$\mathcal{H}_{\text{eff}} = \frac{4t^2}{U} \sum_{\langle i,j \rangle} \left(S_i^z S_j^z - \frac{1}{4} n_i n_j + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \right) \quad (\text{A.34})$$

But $S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) = \mathbf{S}_i \cdot \mathbf{S}_j$ and $n_i = n_j = 1$ in the ground state subspace, so the effective Hamiltonian becomes

$$\mathcal{H}_{\text{eff}} = \frac{4t^2}{U} \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right), \quad (\text{A.35})$$

which corresponds to the antiferromagnetic Heisenberg model: $\mathcal{H}_{\text{Heis}} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$, with $J = 4t^2/U$.

A.6 On the finite temperature Wick's theorem

A product of operators containing k factors c_i^\dagger and $n - k$ factors c_i is brought into *normal ordering* by the operator \mathcal{N} (also written $: \cdot :$) defined as

$$\mathcal{N}[c_1^{(\dagger)} c_2^{(\dagger)} \dots c_n^{(\dagger)}] =: c_1^{(\dagger)} c_2^{(\dagger)} \dots c_n^{(\dagger)} : \equiv (-1)^P c_{i_1}^\dagger c_{i_2}^\dagger \dots c_{i_k}^\dagger c_{i_{k+1}} \dots c_{i_n}, \quad (\text{A.36})$$

where P is the parity of the permutation $1, 2, \dots, n \mapsto i_1, i_2, \dots, i_n$.

It is straightforward to simplify a product of two operators: $C_1 C_2 = \mathcal{N}[C_1 C_2] + \{C_1^-, C_2^+\}$, using the anti-commutation rules. Here C_i^\pm is a combination of fermionic creation (annihilation) operators. The last term is a c-number by assumption. Defining a contraction as $\overline{C_1 C_2} \equiv C_1 C_2 - \mathcal{N}[C_1 C_2]$, we obtain $\overline{C_1 C_2} = \{C_1^-, C_2^+\}$. The definition of a contraction holds even there are other operators between the two contracted ones $C_{1,2}$. Wick's theorem generalizes the result for a product of two operators, giving an expression for the product of an arbitrary number of operators.

Let us state the zero temperature version of Wick's theorem for generic operators $C_i = C_i^+ + C_i^-$.

$$C_1 C_2 \dots C_n = \mathcal{N}[C_1 C_2 \dots C_n] + \sum_{(ij)} \mathcal{N}[C_1 C_2 \dots \overline{C_i \dots C_j} \dots C_n] + \sum_{(ij),(lm)} \mathcal{N}[C_1 C_2 \dots \overline{C_i \dots C_l} \dots \overline{C_j \dots C_m} \dots C_n] + \dots, \quad (\text{A.37})$$

where the first sum is over single contractions of pairs, the second one on double contractions, and so on. For odd n , the last term contains single unpaired operators. Otherwise, they are just products of contractions, which are c-numbers.

A general rule follows from the fact that the average of a normally ordered operator vanishes in the ground state. Two-point correlation functions determine all n -point correlation functions. In particular, for the case of 4 operators, using a self-explanatory abbreviated notation:

$$\langle gs | 1234 | gs \rangle = \langle 12 \rangle \langle 34 \rangle - \langle 13 \rangle \langle 24 \rangle + \langle 14 \rangle \langle 23 \rangle \quad (\text{A.38})$$

Of course, in the finite temperature case, Wick's theorem is not an operator identity because there is no non ambiguous way of defining normal ordering. However, for non-interacting particles, the thermal average of a product of one-particle operators is still a sum over all possible contractions of pairs. All that changes is the definition of the contraction, which is now defined in terms of the thermal average of the product of a pair of operators. Additionally, the theorem generalizes for time-ordered products, simply by replacing the thermal averages of the pair products by time-ordered pair averages.

In particular, for a free theory, the n -particle Green's function, defined by the field operators $\hat{\psi}(x)$,

$$\mathcal{G}(x_1, x_2, \dots, x_n; y_1, y_2, \dots, y_n) \equiv \left\langle \mathcal{T} \hat{\psi}(x_1) \hat{\psi}(x_2) \dots \hat{\psi}(x_n) \hat{\psi}^\dagger(y_1) \hat{\psi}^\dagger(y_2) \dots \hat{\psi}^\dagger(y_n) \right\rangle \quad (\text{A.39})$$

is determined solely by the set of all one-particle Green's functions. Here x and y denote both the complete set of quantum numbers describing the system's degrees of freedom, and imaginary time.

Applying Wick's theorem to the set of non-interacting (and thus independent) particles, we obtain

$$\mathcal{G}(x_1, x_2, \dots, x_n; y_1, y_2, \dots, y_n) = \sum_P (-1)^P \mathcal{G}^0(x_1; y_{i_1}) \mathcal{G}^0(x_2; y_{i_2}) \dots \mathcal{G}^0(x_n; y_{i_n}), \quad (\text{A.40})$$

which corresponds to evaluating the determinant of the matrix \mathbf{G} , defined as $G_{ij} \equiv \mathcal{G}^0(x_i; x_j)$ for $i, j = 1, 2, \dots, n$, where the \mathcal{G}^0 are the free-particle Green's functions, also called propagators.

B

Formulating Auxiliary Field Quantum
Monte Carlo

B.1 Casting the fermionic trace as a determinant

Let the two arbitrary real matrices be \mathbf{M} and \mathbf{N} . Then, a particular case of the identity of Eq.(3.50) is

$$\text{Tr} [e^{-c_i^\dagger M_{ij} c_j} e^{-c_i^\dagger N_{ij} c_j}] = \det(\mathbf{I} + e^{-\mathbf{M}} e^{-\mathbf{N}}), \quad (\text{B.1})$$

where a summation over repeated indices is implied, as it will be throughout this proof.

To prove this identity, we start by proving that

$$e^{-c_i^\dagger M_{ij} c_j} e^{-c_i^\dagger N_{ij} c_j} = e^{-\sum_\nu c_\nu^\dagger \rho_\nu c_\nu}, \quad (\text{B.2})$$

where $\lambda_\nu = e^{-\rho_\nu}$ are the eigenvalues of the matrix $e^{-\mathbf{M}} e^{-\mathbf{N}}$.

The proof consists of showing that any many-particle state are propagated in the same way when acted upon by any of these two operators, i.e. the LHS operator leads the system to the same state as the RHS operator.

A generic single-particle state reads

$$|\phi\rangle = \sum_j a_j c_j^\dagger |0\rangle, \quad (\text{B.3})$$

where a_j are arbitrary coefficients, and $|0\rangle$ is the vacuum state.

Let $\{|\mu\rangle\}$ be the basis in which the matrix \mathbf{N} is diagonal. Using Dirac notation, we then have

$$\mathbf{N} = \sum_\mu |\mu\rangle n_\mu \langle \mu| \quad (\text{B.4})$$

Define new fermionic operators

$$c_\mu = \sum_j \langle \mu | j \rangle c_j \quad c_\mu^\dagger = \sum_j \langle j | \mu \rangle c_j^\dagger, \quad (\text{B.5})$$

which may be inverted to obtain

$$c_j = \sum_\mu \langle j | \mu \rangle c_\mu \quad c_j^\dagger = \sum_\mu \langle \mu | j \rangle c_\mu^\dagger, \quad (\text{B.6})$$

Now we prove yet another identity that goes into proving equation (B.2).

$$e^{-c_i^\dagger N_{ij} c_j} = \prod_\mu [\mathbb{1} + (e^{-n_\mu} - 1)c_\mu^\dagger c_\mu] \quad (\text{B.7})$$

$$\begin{aligned}
\exp(-c_i^\dagger N_{ij} c_j) &= \exp\left(-\sum_{\mu\nu} \langle\mu|i\rangle c_\mu^\dagger N_{ij} \langle j|\nu\rangle c_\nu\right) \\
&= \exp\left(-\sum_{ij} \sum_{\mu\nu\sigma} \langle\mu|i\rangle \langle i|\sigma\rangle c_\mu^\dagger n_\sigma \langle\sigma|j\rangle \langle j|\nu\rangle c_\nu\right), \\
&\quad (\text{using the closure relation } \sum_i |i\rangle \langle i| = \mathbb{1}) \\
&= \exp\left(-\sum_{\mu\nu\sigma} \overbrace{\langle\mu|\sigma\rangle}^{\delta_{\mu\sigma}} c_\mu^\dagger n_\sigma \overbrace{\langle\sigma|\nu\rangle}^{\delta_{\sigma\nu}} c_\nu\right) \\
&= \exp\left(-\sum_\mu c_\mu^\dagger n_\mu c_\mu\right) \\
&= \prod_\mu e^{-n_\mu \hat{n}_\mu} \\
&= \prod_\mu [\mathbb{1} + (-n_\mu \hat{n}_\mu + \frac{n_\mu^2}{2!} \hat{n}_\mu^2 - \frac{n_\mu^3}{3!} \hat{n}_\mu^3 + \dots)] \\
&= \prod_\mu [\mathbb{1} + (-n_\mu + \frac{n_\mu^2}{2!} - \frac{n_\mu^3}{3!} + \dots) \hat{n}_\mu] \\
&\quad (\text{since } \hat{n} = \hat{n}^k \text{ for all } k \in \mathbb{N} \text{ for fermions since } n = 0, 1) \\
&= \prod_\mu [\mathbb{1} + (e^{-n_\mu} - 1) c_\mu^\dagger c_\mu] \quad \square
\end{aligned}$$

Let

$$|\phi\rangle = \sum_j a_j c_j^\dagger |0\rangle \tag{B.8}$$

be an arbitrary many-particle state.

Now we use the previous identity to prove that applying the operator of equation (B.7) to $|\phi\rangle$ we obtain

$$e^{-c_i^\dagger N_{ij} c_j} |\phi\rangle = \sum_j a'_j c_j^\dagger |0\rangle, \tag{B.9}$$

with

$$a'_j = \sum_i (e^{-\mathbf{N}})_{ji} a_i \tag{B.10}$$

We start by writing $|\phi\rangle$ in the basis $\{|\mu\rangle\}$ (in which \mathbf{N} is diagonal).

$$|\phi\rangle = \sum_{i,\mu} a_i \langle\mu|i\rangle c_\mu^\dagger |0\rangle \tag{B.11}$$

Then, we apply the RHS of equation (B.7) to $|\phi\rangle$ written in this basis.

$$\begin{aligned}
& \sum_{\nu} \left[\mathbb{1} + (e^{-n_{\mu}} - 1) c_{\nu}^{\dagger} c_{\nu} \right] c_{\mu}^{\dagger} |0\rangle \\
&= \left[\mathbb{1} + (e^{-n_{\mu}} - 1) c_{\mu}^{\dagger} c_{\mu} \right] c_{\mu}^{\dagger} |0\rangle \\
&= c_{\mu}^{\dagger} |0\rangle + (e^{-n_{\mu}-1} - 1) c_{\mu}^{\dagger} |0\rangle \\
&= c_{\mu}^{\dagger} e^{-n_{\mu}} |0\rangle
\end{aligned} \tag{B.12}$$

$$\begin{aligned}
& \sum_{\nu} \left[\mathbb{1} + (e^{-n_{\mu}} - 1) c_{\nu}^{\dagger} c_{\nu} \right] |\phi\rangle \\
&= \sum_{i\mu} \langle \mu | i \rangle a_i e^{-n_{\mu}} c_{\mu}^{\dagger} \\
&= \sum_{j\mu i} \langle j | \mu \rangle e^{-n_{\mu}} \langle \mu | i \rangle a_i |j\rangle \\
&= \sum_{ji} \underbrace{\sum_{\mu\nu} \langle j | \mu \rangle e^{-N_{\mu\nu}} \langle \nu | i \rangle a_i}_{(e^{-\mathbf{N}})_{ji}} |j\rangle \\
&= \sum_j a'_j c_j^{\dagger} |0\rangle
\end{aligned} \tag{B.13}$$

Similarly, by repeating the procedure performing a change of basis to the eigenbasis of \mathbf{M} , we obtain the more general relation

$$\begin{aligned}
e^{-c_i^{\dagger} M_{ij} c_j} e^{-c_i^{\dagger} N_{ij} c_j} |\phi\rangle &= \sum_j a''_j c_j^{\dagger} |0\rangle \\
a''_j &= \sum_i (e^{-\mathbf{M}} e^{-\mathbf{N}})_{ji} a_i
\end{aligned} \tag{B.14}$$

The amplitude of a propagated state is given by multiplying the initial amplitude by the matrix $e^{-\mathbf{M}} e^{-\mathbf{N}}$, whichever the basis we choose. Then, since equation (B.14) holds in particular for the choice of the eigenbasis of $e^{-\mathbf{M}} e^{-\mathbf{N}}$ as our basis of single-particle states, if we start with an eigenstate

$$|\phi\rangle = c_{\nu}^{\dagger} |0\rangle, \tag{B.15}$$

then the amplitude of the propagated state will be given by

$$(e^{-\mathbf{M}} e^{-\mathbf{N}})_{\nu\nu} = e^{-\rho_{\nu}}, \tag{B.16}$$

the same as we would obtain from equation (B.2). Clearly, if we start with a state that is an arbitrary combination of states of the eigenbasis, we would obtain the identity (B.2).

The identity was proven for a single-particle state. Does it generalize to more than one particle? As we did before, we start with propagation by a single factor $e^{-\mathbf{N}}$. Take a two-particle state

$$|\phi\rangle = c_{\mu_1}^{\dagger} c_{\mu_2}^{\dagger} |0\rangle \tag{B.17}$$

Now propagate it with \mathbf{N} , i.e.

$$\begin{aligned} e^{-c_i^\dagger N_{ij} c_j} |\phi\rangle &= \prod_\mu \left[1 + (e^{-n_\mu} - 1) c_\mu^\dagger c_\mu \right] c_{\mu_1}^\dagger c_{\mu_2}^\dagger |0\rangle \\ &= e^{-n_{\mu_1}} e^{-n_{\mu_2}} c_{\mu_1}^\dagger c_{\mu_2}^\dagger |0\rangle, \end{aligned} \quad (\text{B.18})$$

where we simply note that by similar reasoning to the previous case, we would in equation (B.12) keep two terms corresponding to $\mu_1 \neq \mu_2$. If $\mu_1 = \mu_2$, then both sides are equal to zero due to Pauli's exclusion principle and the equality holds trivially. This reasoning clearly generalizes to an arbitrary superposition of many-particle states. Moreover, we proved the result for a product of two factors $e^{-\mathbf{M}} e^{-\mathbf{N}}$, but it is also easy to see that by successive changes of basis, we could extend our result to an arbitrary number of factors.

To complete our proof of the identity (B.1) that is so crucial in formulating AFQMC, we use the auxiliar identity we just proved (B.2).

$$\begin{aligned} \text{Tr} \left[e^{-\sum_\nu c_\nu^\dagger \rho_\nu c_\nu} \right] &= \text{Tr} \left[\prod_\nu e^{-c_\nu^\dagger \rho_\nu c_\nu} \right] \text{ since } [\hat{n}_\mu, \hat{n}_\nu] = 0 \\ &= \prod_\nu (1 + e^{-\rho_\nu}) = \det[\mathbf{I} + e^{-\mathbf{M}} e^{-\mathbf{N}}], \quad \square \end{aligned} \quad (\text{B.19})$$

where the last equality stems from the fact that the determinant of a diagonal matrix is just the product of the eigenvalues.

B.2 Rank-one updates of the Green's function

Consider two matrices $\mathbf{A}_1, \mathbf{A}_2$ written in the form

$$\mathbf{A}_{1,2} = \mathbf{I} + \mathbf{F} \mathbf{V}_{1,2}, \quad (\text{B.20})$$

where \mathbf{F} is some matrix. $\mathbf{V}_{1,2}$ are diagonal and non-singular and differ only in the $(1, 1)$ entry, so that

$$\mathbf{V}_1^{-1} \mathbf{V}_2 = \mathbf{I} + \alpha_1 \mathbf{e}_1 \mathbf{e}_1^T, \quad (\text{B.21})$$

where \mathbf{e}_1 is a vector corresponding to the first column of the identity matrix \mathbf{I} , and

$$\alpha_1 = \frac{V_2(1, 1)}{V_1(1, 1)} - 1 \quad (\text{B.22})$$

Then, \mathbf{A}_2 is clearly a rank-one update of \mathbf{A}_1 .

$$\begin{aligned} \mathbf{A}_2 &= \mathbf{I} + \mathbf{F} \mathbf{V}_1 + \mathbf{F} \mathbf{V}_1 (\mathbf{V}_1^{-1} \mathbf{V}_2 - \mathbf{I}) \\ &= \mathbf{A}_1 + \alpha_1 (\mathbf{A}_1 - \mathbf{I}) \mathbf{e}_1 \mathbf{e}_1^T \\ &= \mathbf{A}_1 [\mathbf{I} + \alpha_1 (\mathbf{I} - \mathbf{A}_1^{-1}) \mathbf{e}_1 \mathbf{e}_1^T] \end{aligned} \quad (\text{B.23})$$

To find an expression for the ratio of the determinants of \mathbf{A}_1 and \mathbf{A}_2 , we shall need to make use of the Sylvester's determinant identity $\det(\mathbf{I} + \mathbf{AB}) = \det(\mathbf{I} + \mathbf{BA})$. To prove it, consider the matrices

$$\mathbf{P} = \begin{pmatrix} \mathbf{I} & -\mathbf{A} \\ \mathbf{B} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{A} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \quad \mathbf{Q} = \begin{pmatrix} \mathbf{I} & \mathbf{A} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{I} & -\mathbf{A} \\ \mathbf{B} & \mathbf{I} \end{pmatrix} \quad (\text{B.24})$$

Using the identity $\det(\mathbf{AB}) = \det(\mathbf{A}) \det(\mathbf{B})$ applied to these two matrices, we can clearly see that the determinants of the two matrices coincide, i.e.

$$\det(\mathbf{P}) = \det \begin{pmatrix} \mathbf{I} & -\mathbf{A} \\ \mathbf{B} & \mathbf{I} \end{pmatrix} \det \begin{pmatrix} \mathbf{I} & \mathbf{A} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \quad \det(\mathbf{Q}) = \det \begin{pmatrix} \mathbf{I} & \mathbf{A} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \det \begin{pmatrix} \mathbf{I} & -\mathbf{A} \\ \mathbf{B} & \mathbf{I} \end{pmatrix} \quad (\text{B.25})$$

The sought identity is obtained by computing the determinants explicitly.

$$\det(\mathbf{P}) = \det \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{B} & \mathbf{I} + \mathbf{BA} \end{pmatrix} = \mathbf{I} + \mathbf{BA} \quad \det(\mathbf{Q}) = \det \begin{pmatrix} \mathbf{I} + \mathbf{AB} & \mathbf{0} \\ \mathbf{B} & \mathbf{I} \end{pmatrix} = \mathbf{I} + \mathbf{AB} \quad (\text{B.26})$$

A corollary of Sylvester's identity for any two column vectors: $\det[\mathbf{I} + \mathbf{xy}^T] = 1 + \mathbf{y}^T \mathbf{x}$ may be used with $x \mapsto (\mathbf{I} - \mathbf{A}_1^{-1})\mathbf{e}_1$, $y \mapsto \mathbf{e}_1$ to write the ratio of the determinants of matrices \mathbf{A}_1 and \mathbf{A}_2 as

$$r_1 = \frac{\det[\mathbf{A}_2]}{\det[\mathbf{A}_1]} = 1 + \alpha_1(1 - \mathbf{e}_1^T \mathbf{A}_1^{-1} \mathbf{e}_1), \quad (\text{B.27})$$

which reduces the computation of the ratio r_1 to computing the (1,1) entry of \mathbf{A}^{-1} .

Now we generalize this idea for a sequence of matrices $\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_i, \dots, \mathbf{A}_n$ generated by successive rank-one updates: $\mathbf{A}_{i+1} = \mathbf{I} + \mathbf{FV}_{i+1}$, $i = 1, 2, \dots, n-1$, with

$$\mathbf{V}_i^{-1} \mathbf{V}_{i+1} = \mathbf{I} + \alpha_i \mathbf{e}_i \mathbf{e}_i^T \quad \alpha_i = \frac{\mathbf{V}_{i+1}(1,1)}{\mathbf{V}_i(1,1)} - 1 \quad (\text{B.28})$$

That is accomplished by use of the Sherman-Morrison-Woodbury formula, or simply Woodbury matrix identity:

$$(\mathbf{A} + \mathbf{BCD})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1} \mathbf{B} (\mathbf{C}^{-1} + \mathbf{DA}^{-1} \mathbf{B})^{-1} \mathbf{DA}^{-1}, \quad (\text{B.29})$$

where $\dim(\mathbf{A}) = N \times N$, $\dim(\mathbf{B}) = N \times K$, $\dim(\mathbf{C}) = K \times K$, $\dim(\mathbf{D}) = K \times N$, and N and K are integers. To prove the identity, we use two simple identities, from which the proof easily follows.

$$\mathbf{B} + \mathbf{BCDA}^{-1} \mathbf{B} = (\mathbf{A} + \mathbf{BCD}) \mathbf{A}^{-1} \mathbf{B} \quad (\mathbf{A} + \mathbf{BCD})^{-1} \mathbf{BC} = \mathbf{A}^{-1} \mathbf{B} (\mathbf{C}^{-1} + \mathbf{DA}^{-1} \mathbf{B})^{-1} \quad (\text{B.30})$$

$$\begin{aligned} \mathbf{A}^{-1} &= (\mathbf{A} + \mathbf{BCD})^{-1} (\mathbf{A} + \mathbf{BCD}) \mathbf{A}^{-1} = (\mathbf{A} + \mathbf{BCD})^{-1} (\mathbf{I} + \mathbf{BCDA}^{-1}) \\ &= (\mathbf{A} + \mathbf{BCD})^{-1} + (\mathbf{A} + \mathbf{BCD})^{-1} \mathbf{BCDA}^{-1} \\ &= (\mathbf{A} + \mathbf{BCD})^{-1} + \mathbf{A}^{-1} \mathbf{B} (\mathbf{C}^{-1} + \mathbf{DA}^{-1} \mathbf{B}) \mathbf{DA}^{-1} \quad \square \end{aligned} \quad (\text{B.31})$$

The Woodbury identity applied to Eq.(B.23) gives an expression for \mathbf{A}_2^{-1} as a rank-one update of \mathbf{A}_1^{-1} .

$$\begin{aligned}\mathbf{A}_2^{-1} &= \mathbf{A}_1^{-1} - \alpha_1(\mathbf{I} - \mathbf{A}_1^{-1}) \underbrace{\left[\mathbf{e}_1 + \mathbf{e}_1^T \mathbf{A}_1^{-1} \alpha_1 (\mathbf{A}_1 - \mathbf{I}) \right]}_{\mathbf{e}_1 \times, \times \mathbf{e}_1 \text{ (multiply left and right)}}^{-1} \mathbf{e}_1^T \mathbf{A}_1^{-1} \\ &= \mathbf{A}_1^{-1} - \alpha_1(\mathbf{I} - \mathbf{A}_1^{-1}) \mathbf{e}_1 \left[1 + \alpha_1(1 - \mathbf{e}_1^T \mathbf{A}_1^{-1} \mathbf{e}_1) \right]^{-1} \mathbf{e}_1^T \mathbf{A}_1^{-1} \\ &= \mathbf{A}_1^{-1} - \frac{\alpha_1}{r_1} \mathbf{u}_1 \mathbf{w}_1^T,\end{aligned}\tag{B.32}$$

where the operation on the first step does not affect the term in parentheses, and we defined $\mathbf{u}_1 = (\mathbf{I} - \mathbf{A}_1^{-1}) \mathbf{e}_1$ $\mathbf{w}_1 = (\mathbf{A}_1^{-1})^T \mathbf{e}_1$.

Using Eqs.(B.27,B.32) successively, we find the updates

$$\begin{aligned}r_i &= \frac{\det[\mathbf{A}_{i+1}]}{\det[\mathbf{A}_i]} = 1 + \alpha_i(1 - \mathbf{e}_i^T \mathbf{A}_i^{-1} \mathbf{e}_i), \text{ and} \\ \mathbf{A}_{i+1}^{-1} &= \mathbf{A}_i^{-1} - \frac{\alpha_i}{r_i} \mathbf{u}_i \mathbf{w}_i^T,\end{aligned}\tag{B.33}$$

where $\mathbf{u}_i = (\mathbf{I} - \mathbf{A}_i^{-1}) \mathbf{e}_i$ and $\mathbf{w}_i = (\mathbf{A}_i^{-1})^T \mathbf{e}_i$.

It is possible to generalize this procedure to compute the inverse of \mathbf{M}_k as a rank- $(k-1)$ update of \mathbf{A}_1^{-1} to devise a delayed update scheme that is more efficient:

$$\mathbf{M}_k^{-1} = \mathbf{M}_1^{-1} - \mathbf{U}_{k-1} \mathbf{D}_k \mathbf{W}_{k-1}^T,\tag{B.34}$$

where

$$\mathbf{U}_k = [\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_{k-1}] \quad \text{and} \quad \mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_{k-1}],\tag{B.35}$$

and $\mathbf{D}_k = \text{diag}(\alpha_1/r_1, \alpha_2/r_2, \dots, \alpha_{k-1}/r_{k-1})$.

In [88], precise bounds are given on the conditioning of the matrices obtained via such type of Sherman-Morrison updates. In practice, if the Green's functions are sufficiently well-conditioned, no precision-related issues arise. Numerical instabilities may arise when the Green's matrices comprise divergent energy scales, and care must be taken to ensure that the algorithm converges.

