Correlation effects in low dimensional quantum systems: From Ladders to 2D Materials

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Dedication

To my parents, Sheng Wan Yang and Jie Wang, who gave me life and passed on a love of reading and respect for education. Without their caring support and sacrifice, this work would not have been possible.
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Abstract of Dissertation

This dissertation discussed four low-dimensional systems: Hubbard ladder and its 2D extension, anisotropic Hubbard ladder, one-dimensional two-orbital t-J model, and Kondo model. All of them are of strongly correlated.

Doped cuprates, as strongly correlated systems, have attracted a lot of attention in the condensed matter physics community, not just from the purely theoretical perspective, but also due to the novel applications beyond the conventional semiconductor paradigm. They display complicated phase diagram, defying the conventional rigid band theory, shaking our common sense and driving us to wrestle with many-body physics. With the aid of advanced experimental techniques such as ARPES, its various exotic electronic structure, such as waterfalls, hole pockets, Fermi arcs and kinks have been unveiled and remain open to interpretation. To attack such complicated problems, people usually build various models to mimic the CuO$_2$ planes, which is the common feature of various cuprate compounds and is believed to be mainly responsible for their complicated properties, especially the high temperature superconductivity. In Chapter 3, we simulated the spectral properties of the 2-leg single-band Hubbard ladder and its 2-dimensional extension at and away from half-filling using the numerical tool: the combination of Cluster Perturbation Theory (CPT) with the time-dependent density matrix renormalization group method (tDMRG) as a solver. The main features of the spectrum can be described with a mean-field dispersion, with kinks and pseudogap traced back to scattering between spin and charge degrees of freedom. As a bonus, we find that the spectrum of hubbard ladder involves spin-polaron, the bound state of spinon and holon.

Interacting one-dimensional electron systems generically behave different from higher dimensional systems in the sense that its low-energy excitations are described by Luttinger liquid theory as collective bosonic modes carrying spin and charge separately, the so-called spinons and holons, rather than the coherent quasi-particles in Fermi liquid theory. This phenomenon is known as spin-charge separation, an intrinsic property of 1D system. It can be thought of as a particular case of electron fractionalization. When multiple 1D chains get coupled, how the picture changes? In Chapter 4, we study the spectral function of the anisotropic 2-leg Hubbard ladder, one of the simplest multiple-chain systems. The spectrum can be understood as the scattering resultants of spinon and holons: As the inter-chain hopping is increased, the continuum in the bonding channel moves to higher energies and spinon and holon branches merge into a single coherent quasi-particle band. Simultaneously, the spectrum undergoes a crossover from a regime with two minima at incommensurate values of $k_x$ (a Mott insulator), to one with a single minimum at $k_x = \pi$ (a band insulator). In addition, the spectrum contains a continuum of scattering states consisting of a triplon and a polaron, accompanied by the formation of bound states with higher spin $\frac{3}{2}$, ferromagnetic “spin bags” in which the hole can move freely.
To analyze the formation of quasi-particle, we study the time-evolution of charge and spin degrees of freedom in real space after a hole is injected, which indicates that incoherent holons and spinons can emerge into polarons, that can propagate coherently, after a characteristic time $\tau$.

Multiorbital systems can involve Mott and Hund physics, and are rich in various phenomena, including orbital selective Mott transitions, spin-orbital separations, and pairing density wave due to the complex interplay between spin, charge and orbital degrees of freedom. Therefore, it can capture many unique features in real strongly correlated systems, such as iron pnictides and ruthenates, and thus attract a lot of investigations. In Chapter 5, we comprehensively study a one-dimensional two-orbital model at and below quarter filling, which realizes a number of unconventional phases, by means of DMRG and some analytical calculations. In particular, we find that the system supports an extensive density wave in which excitons quasicondense with finite center-of-mass momentum. In this phase, excitons behave as hard-core bosons without charge order. In addition, excitons can pair to form biexcitons in a state that is close to a charge density wave instability. Finally, a genuine orbital-selective paired state (metallic plus spin-gapped superconductor) can be realized when pairing dominates over the interorbital repulsion.

Kondo problem, as one of the most studied and best understood correlated systems, has been studied by various techniques, but the internal structure of its ground state has two deeply conflicting pictures: At strong coupling limit, the system is essentially composed of a scattering center, which is a tightly bound singlet formed by the impurity and a localized electron at $r_0$, and the remaining conduction electrons that are decoupled to the impurity and remain almost “free”. At weak enough couplings, the singlet extends to the entire volume and the impurity will couple mostly to one electron at the Fermi level. In chapter 6, we provide a coherent picture to unveil the puzzle in the context of quantum information theory by deconstructing the Kondo singlet, both in real and energy space, and measuring the spin correlations between the impurity and the invididual free electron eigenstate based on two different measures. As a bonus, we can identify “projected natural orbitals” that can be used as a “good” approximate wavefunctions for simulations, and a quasi-order parameter that determines the crossover from weak to strong coupling regimes and furthermore offers the means to measure the Kondo screening length $\zeta_K$. This screening length might be used to characterize the “size” of the Kondo cloud.
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Chapter 1

Introduction

Condensed matter physics describes and predicts the physical properties of many-body systems, which usually involve a macroscopically large number of degrees of freedom. Although we know the constituents and the physical laws governing their motion, it is practically impossible to find the solution to the equations of motion for every constituent. In fact, seeking such solutions of the system is not what we mean by understanding the physics of such many-body system. The properties we really care about are various correlations among observable properties of the system that can be experimentally tested. Such correlations usually can be captured by the low-energy excitations of the system, which might obey some simpler physical laws compared to the original constituents. For instance, the lowest-energy excitations in a crystal correspond to collective modes, called phonons, that represent noninteracting (or weakly coupled) bosonic quasiparticles. Physically, they are quanta of collective motion of atoms or ions in the crystals but provide a much simpler context to characterize the low-temperature lattice properties, meaning that we can obtain various properties of the crystal lattice in terms of these effective degrees of freedom without resorting to the underlying interacting constituents. Technically, we can build up low-energy effective theory containing phonons to describe the low-temperature lattice properties.
Fermi liquid theory [14], one of the paradigmatic effective theories, constitutes one of the two pillars of “standard model” in condensed matter physics. It helps us understand quasi-particles and collective excitations in metals, building on a continuous link between a non-interacting and an interacting system, and provides the foundation for many condensed matter problems, especially 3D systems: the quasi particle excitations within this theory have the same quantum numbers as the electron with charge $e$, spin $\frac{1}{2}$ and momentum, but move with a “renormalized” velocity, or mass. The important characteristics of the excitations of Fermi liquid are shown in Fig.1.1. Simply stated, it establishes a one-to-one correspondence between quasi-particles in the interacting system and the free electrons of the system, which is referred to as the “adiabatic approximation”. Compared to free electrons, quasi-particles are essentially electrons dressed by the particle-hole excitations. As a bonus, the Fermi liquid theory indicates that quasi-particles can be treated as almost-free, independent entities approximately and the residual mutual interactions just play a role of “weak perturbation”. On top of that, conventional band theory provides a single-particle picture in the presence of crystal lattice structure and has achieved remarkable successes in characterizing and understanding electronic structures and various properties of a large amount of materials including most band insulators and semiconductors. It has yielded many important discoveries, such as the transistors that form the foundation of our current technology.

1.1 Rich physics beyond Fermi liquid theory and band theory

If many-body systems could always be treated in a single-particle picture, the world would be very boring. As Aristotle once said: “The whole is greater than the sum of its parts”, and that’s certainly true in condensed matter physics: Interactions and correlations among particles can yield a qualitative change of the whole system.
Figure 1.1: a). The occupation \( n(k) \) of free electrons is a step function with discontinuity at the Fermi surface \( k = k_F \). c). The spectral function of free electrons is just a delta function peak, showing excitations without damping and a well-defined dispersion. This means the excitations are made of the individual particles of a given momentum. b). The occupation \( n(k) \) of Fermi liquid still displays a discontinuity at the Fermi surface, but with a reduced amplitude \( Z < 1 \). Accordingly, some states above the Fermi surface are occupied due to the leakage of occupation below and close to the Fermi surface. d). The spectral function of Fermi liquid consists of additional excitations far below the Fermi surface, in addition to a single peak near the Fermi surface corresponding to the quasi-particle in Fermi liquid theory. From [1]

As a matter of fact, there are a lot of materials that can not be understood in the context of Fermi liquid theory and band theory.

1.1.1 Dimensionality: The fate of Luttinger liquid theory

In spite of success of Fermi liquid theory in high-dimensional systems, it breaks down in one-dimensional (1D) systems [1]: the low-energy excitations in 1D are described by Luttinger liquid theory as collective bosonic modes carrying spin and charge separately, the so-called spinon and holon, which is known as spin-charge separation, an intrinsic property of 1D systems. In the nutshell, a fermion injected into such systems breaks down into excitations carrying different quantum numbers, each with a characteristic energy scale and velocity. This physical process can be schematically illustrated in Fig.1.2. The Luttinger liquid theory provides a complementary picture of condensed matter physics, which is consistent with the intuition that electrons cannot move without encountering other electrons in one-dimensional system and only collective motions are available.
Figure 1.2: Cartoon description of spin-charge separation on a single chain: a). The half-filled case is assumed to display quasi-antiferromagnetic (AFM) order; b). The quasi AFM order can be locally disrupted once doped with a hole; c). When the hole moves, a spin domain wall, called spinon, is left behind; d). The hole can move via the conventional hopping process, determined by \( t \); e). The spinon can “hop” by two sites for each spin flip. This process is governed by the spin-spin coupling \( J \).

**Experimental realization**: The peculiar one-dimensional behavior was firstly realized in isolated 1D and later in bulk materials with polymers and organic compounds. Some of them are organic superconductors, ladder compounds, quantum wires, carbon nanotubes, edge states in quantum hall systems. As an example, TTF-TCNQ (Tetrathiafulvalene-tetracyanoquinodimethane) is a quasi-1D organic conductor whose crystal structure is shown in Fig.1.3 from Ref.[2]. Another example of a 1D-type material representing spin-charge separation is \( SrCuO_2 \), whose crystal structure is shown in Fig.1.4. This material is effectively treated as one-dimensional since the intrachain hopping is quite large compared to the interchain hopping.

**Why 1D is peculiar**: In the following, we will simply explain the origin of the discrepancy between 1D and higher dimensions. The absence of quasi-particles in 1D can be signaled by the unconventional analytic structure of the associated single-particle Green’s function in 1D: the generic single-particle Green’s function in \( D>1 \) has poles, among which the one with lowest energy corresponds to the quasi-particles, while the 1D correspondence has branch cuts instead of poles [15],

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meaning that it has no well-defined quasi-particles. For instance, in the special case where spin and charge have the same velocity, the Green’s function has a rather simple formula

\[ G(\omega, q) = -\frac{Z_0}{\omega - vq} \left[ \frac{m}{\sqrt{m^2 + v^2 q^2 - \omega^2}} - 1 \right] \]

where \( Z_0 \) is related to the single-particle residue and \( m \) represents the gap. Obviously, it has no poles but only branch cuts as expected. Compared to the

\[^{1}\text{Note that this still fulfills the Luttinger theorem, which relates the particle density } n \text{ to the surface restricted by singularities of } \ln G(\omega = 0, p), \text{ which don’t distinguish between infinities and zeros of } G(\omega = 0, p)\]
noninteracting case in which the Green’s function has well-defined pole corresponding to the free particles, any finite-order perturbation approaches fail to reproduce such analytic structure of Green’s function.

As mentioned above, the low-energy excitations in 1D interacting system should be collective modes since single particles ineluctably hinder each other. We can measure these collective modes by calculating some particular two-particle Green’s functions such as the density-density correlation functions in the perturbation theory. As an example, the polarization tensor (also known as the susceptibility) in the particle-hole channel to the leading order is given by

\[
\chi(q, \omega) = \frac{1}{\Omega} \sum_p \frac{f_F(\epsilon_p) - f_F(\epsilon_{p+q})}{\omega + \epsilon(p) - \epsilon(p + q) + i\delta}
\]

where \( \Omega \) denotes the volume of the system, \( f_F \) represents the Fermi-Dirac distribution and \( \epsilon(p) \) corresponds to the dispersion of free particles. At low temperature and energy, only states near the Fermi surfaces are important. In 1D system, the dispersion (shown in Fig.1.5) can be linearized,

\[
\epsilon(k) \approx \begin{cases} 
  v_F(k - k_F) & \text{if } k \sim k_F \\
  v_F(-k - k_F) & \text{if } k \sim -k_F 
\end{cases}
\]

obeying the nesting condition \( \epsilon(k + 2k_F) = -\epsilon(k) \). Compared to the higher-dimensional Fermi surfaces, 1D Fermi surface is generically nested, regardless of the precise dispersion. We can easily find that the static polarization has a logarithmic divergence at \( q = 2k_F \) (as shown in Fig.1.6) contributed from the particle-hole in the backward channel:

\[
\chi(q, 0) \sim \ln \frac{\Lambda}{2k_F - q} \quad q \sim 2k_F
\]

where \( \Lambda \) is a cutoff introduced to represent the range within which the linearized dispersion holds. So the singular behavior of the static \( \chi \) in the weak coupling of
Figure 1.5: Nesting properties of Fermi surfaces. a). In one dimension, the Fermi surface consists of only two points and is totally nested. Near the Fermi point, the dispersion can be linearized (blue line). The associated nesting wavevector $Q$ is $2k_F$. b). Nesting occurs in some particular case, for instance, a square Fermi surface in two dimension. In this case, the nesting wavevector is $Q = (\pi, \pi)$. From [1].

1D system results from the perfect nesting feature of Fermi surface and leads to the so-called Peierls instability: In 1D case, the nesting feature is pervasive on the whole Fermi surface enhancing the singularity. In addition, the polarization corresponds to the vertex correction, so this logarithmic enhancement at $Q = 2k_F$ yields an effective and relevant interaction involving finite momentum transfer $Q = 2k_F$. This is quite different from the Fermi liquid theory, where the interactions involving momentum transfer are irrelevant, and finally generates spin-charge separation [16].

Figure 1.6: Schematical illustration of the polarization tensor in different dimensional systems: a). The singularity of the denominator is smoothed over in 3d systems. b) and c). The singularities in lower (2d and 1d) dimensional system are enhanced further. In the 1d case, the polarization itself has a logarithmic divergence, which leads to instabilities of 1d metals, at $q = 2p_F$. As expected, the static polarization $\chi(q,0)$ exquisitely depends on the dimensionality via the geometry and topology of Fermi surface.
Exceptions in 1D: It should be kept in mind that there are exceptions [17] in 1D that cannot be described as Luttinger liquid theory, although the latter is quite dominant in 1D. Two known examples are Mott insulator and Luther-Emery liquid: Mott insulator is induced by the umklapp processes, whose couplings goes to strong in the half-filled case and generates a gap in the excitation spectrum, so this phase has a charge gap but its spin sector remains gapless. Luther-Emery liquid is contributed from the backward scattering, which generates a spin gap and keeps the charge excitation gapless. Note that both phases can be realized in Hubbard model with repulsive and attractive $U$, respectively.

Unsolved problems: Given “standard models” for 1D and high-dimensional systems in condensed matter physics, many questions still remain open. For instance, when multiple 1D systems get coupled, how this physical picture changes: What the fate of these density fluctuations is and how quasiparticles emerge, have been studied extensively. More generally, what kinds of new excitations can arise in lower-dimensional systems, or equivalently, what is in between these two oases (Luttinger Liquid and Fermi Liquid theories), deserts or more oases?

1.1.2 Strong interaction: Mott physics

When the Coulomb repulsion is too strong or the bandwidth is too narrow, the single-particle picture might break down as well. Such systems are called Mott-insulators, whose properties can not be appropriately described by band theory, since their behavior is governed by complicated many-body interactions and correlations. For instance, $NiO$ should be metal according to the band theory, since it has partially filled band. But the strong electron-electron repulsion brings about the multiple-electron correlation yielding the breakdown of normal band properties for the $d$ electrons as indicated by Mott [18]: The strong coupling induces a new energy gap,
called the Mott gap and electrons tend to be localized, since the relatively high-energy charge fluctuations are effectively blocked. As a consequence, NiO behaves as an insulator.

The introduction of correlations actually implies that the wave function of the system becomes effectively many-body-like, and the one-particle picture and rigid band theory become fragile. As a result, we have to wrestle with real many-body problems. Despite of these difficulties, understanding these materials has attracted a lot of attention in the condensed matter physics community, not just from the purely theoretical perspective, but also due to the novel potential applications beyond the semiconductor paradigm, particularly sparked by the unexpected discovery of high temperature superconductivity (HTSC) in lightly doped antiferromagnets, whose normal-state properties reflected a breakdown of the Landau paradigm as proposed by Philip W. Anderson [19], and many others.

**High-$T_c$ materials are essentially 2D systems** : Generally, high-$T_c$ materials have complicated constituents, but their structures exhibit a common feature, namely they contain weakly coupled copper-oxide planes, which are composed of coplanar copper and oxygen ions and are relatively well separated by the other components, that are rather inert and essentially play the role of charge reservoir. It was assumed that these materials as electronic systems are essentially two-dimensional and the principal actor is the $CuO_2$ plane, which is the key ingredient in cuprates to be responsible for their complicated properties, especially the high temperature superconductivity.

**Progress and unsolved problems** : The “undoped” parent cuprate compounds are assumed to be Mott insulators with long-range antiferromagnetic order at low enough temperature (or charge transfer insulator). Once doped, they usually display complex phase diagrams (as shown in Fig.(1.7)). With the rapid development
of new experimental technologies during the past several decades, their interesting properties have been progressively and continuously revealed. Although much progress has been achieved and a lot of puzzles have been clarified, a full picture about their phases remains lacking. For instance, in the pseudogap regime of the cuprates an order parameter cannot be clearly identified and remains mystery. Even the normal state of the cuprates, called strange metal, displays abnormal transport properties, flouting the norm of physics and attracting a lot of attention. With the aid of various advanced experimental techniques such as angular-resolved photoemission spectroscopy (ARPES), exotic electronic structure of cuprates, such as waterfalls, hole pockets, Fermi arcs and kinks [9, 10, 20, 21], have been revealed and remain open to interpretation.

Figure 1.7: Schematic doping phase diagram of cuprate high-temperature superconductors for both electron and hole doping from wiki.

Spin-polaron approach–Nagaoka type vs. string type: There have hitherto been many theoretical approaches to the HTSC problem. Most of them have emphasized the importance of the experimentally observed magnetism in the parent materials and of the AF spin fluctuations within the superconducting state. Among these efforts, the spin-polaronic approach has played a prominent role in understanding the basic effects of interplay between the spin and charge degrees of freedom in CuO$_2$ planes. In the following, we will briefly overview the spin-polaron concept based on Ref. [22].
It is widely known that the movement of a charge carrier in an ionic lattice is always accompanied by displacement of the ions due to the Coulomb interaction. Under certain conditions, the carrier plus these displacements can form a well-defined quasi-particle, called (charge) polaron. Similarly, when a charge carrier moves in a magnetic medium, the derivation of spin orientation of these localized spins can form a quasi-particle, called spin-polaron, with the propagating charge. The origin of the spin-polaron concept can be traced back to the early work [23] on the “double-exchange” mechanism in manganese oxides, in which doping introduces an effective exchange interaction and resulting in two neighboring Mn spins being aligned. Later, it was found [24] that the mobile carrier can lead to a polarization of the localized antiferromagnetic spins, which make it possible to form spin-polaron. The big progress was achieved after Nagaoka’s study [25] on the single-band Hubbard model with nearly half-filling: the system will have a ferromagnetic (FM) ground state if the on-site repulsion $U$ is infinite. This can be understood as follows: If $U = \infty$, the ground state of the system displays an AFM order. When an extra electron with down spin is injected into it, it cannot move if spin flips around it are forbidden. However, if the energy to flip a spin is small, i.e. the kinetic energy dominates, the electron may lower its kinetic energy enough to compensate for the spin-flip energy and form a ferromagnetic “bubble” called “ferron”. As illustrated in Fig.1.8, the spins become ferromagnetically aligned with one another and antiferromagnetically aligned with the spin of the added electron to form the spin-polaron, called the Nagaoka-type spin-polaron, whose volume determines the energy cost of the polarization. In the Nagaoka limit, the ferron extends to the whole system, i.e. all the spins are polarized and the system displays FM order. Moreover, the Nagaoka-type spin-polaron can have higher spins.

If the added electron can form a tightly bound singlet state with the localized spin, a different type of spin-polaron can form (as shown in Fig.1.9). The movement of hole disrupts the perfect AF order and creates an effective 1D string potential, leading to the confinement of the hole and the formation of the string-type spin-polaron,
Figure 1.8: Cartoon description of the formation of the Nagaoka-type spin-polaron: The doped electron can move, once electrons around it are flipped. As a result, it was confined in a ferromagnetic bubble, called “ferron”, within which the added electron can freely move.

i.e. the spin-polaron oscillates around its origin. Note that the spin of the string-type spin-polaron must be $\frac{1}{2}$, which is an essential difference from the Nagaoka-type spin-polaron.

Figure 1.9: Cartoon description of the formation of the string spin-polaron: The formation of singlet effectively introduce a hole within the AFM array. It can move without flipping a spin since either the singlet spins can pair with the nearest neighbor spins as needed, depending on the orientation of that neighbor. But a string of spins misaligned relative to the initial AF ordering is left behind the hole. Here the dot lines denote the “wrong” bonds increasing the energy.

The parameter range favorable for Nagaoka and string-like polarons have been estimated [26] by comparing their energies. And it was found that if $\frac{t}{J} > 50$, the Nagaoka polaron has lower energy; otherwise, the string polaron is a more favorable excitation. When the spin-polaron concepts are applied to the HTSC, which has strong on-site interaction, the string-type spin polaron is a good candidate, although the Nagaoka-type spin polaron was used to analyze the HTSC in the earlier days. We should keep in mind that the string of misaligned spins can be repaired locally.
due to spin flipping within the “string” and yielding spin-polaron propagation via a higher order processes. This has been confirmed by ARPES data for $Sr_2CuO_2Cl_2$.

1.1.3 Orbital degree of freedom: Hund physics and more

In many real materials, such as iron-based superconductors and ruthenates, relevant electrons might come from multiple orbitals and yield complex phenomenologies such as orbital selective behavior, various orbital orders, due to the interplay between spin, charge and orbital degrees of freedom. In the last few years, there has been increasing awareness that Hund’s coupling may be responsible for these correlations: It drives the system away from the Mott transition but makes the metallic state more correlated by lowering the quasiparticle coherence scale as summarized by Georges [27]. But even without Hund coupling, the intertwine among spin, charge and orbital degrees of freedom can yield interesting physics, such as “spin-orbital separation”, where the excitation of orbitals can decouple from the spin. It can be expected that multiple-orbital systems with strong correlations form unexplored goldmines and deserve further investigation.

1.2 Hubbard Models and their application to HTSC

To illustrate major characteristics of interacting electrons, we usually adopt some idealized models, which are prototypes that bring out features occurring in real problems and ignore irrelevant details.

1.2.1 Hubbard models

The Hubbard model [28] is one of the simplest models for interacting electrons on a lattice, a paradigmatic model in condensed matter physics. It contains the basic ingredients to understand the physics of strongly correlated systems and accounts
for the competition between the delocalization induced by the kinetic energy and the localization due to the on-site Coulomb interaction. Despite its relative simplicity, the physics captured by Hubbard model is quite rich: it can give rise to insulating, magnetic, and superconducting effects in a solid. For instance, it can describe transition between metals and insulators: In the non-interacting limit, it reduces to the tight-binding model which can describe ordinary metals; for strong interaction, the ground state at half-filling is insulating, with one electron per site that is localized. This state is referred-to as a Mott insulator, and at finite coupling is also an antiferromagnet. At finite doping, the model can realize pairing, phase segregation and stripes. As a matter of fact, it has been used to describe the electronic properties of solids with narrow bands, magnetism in iron, cobalt, nickel, and the Mott metal-insulator transition. More interestingly, it has been assumed for decades to be the minimal model for high temperature superconductivity, and has acquired a lot of attention recently, including the efforts to realize it in cold atomic physics. If longer-range hopping, interactions, and/or multiple bands are taken into account, the associated variants can be called generalized Hubbard models, which usually describe more interesting phenomena and contain richer physics. So far, no fully consistent treatment of the Hubbard model is available in general. There are, however, two non-trivial exceptions in which the model can be solved in a sense that many properties are calculable, namely the one- and infinite-dimensional cases.

In the following, we will overview basic properties of single-band Hubbard model, particularly focusing on the one-dimensional case to see how spin-charge separation emerges from the theory.

**The power of on-site Coulomb repulsion–band splitting**: One of the central results about the Hubbard model was that in an array of one-electron atoms with non-degenerate orbitals, the on-site Coulomb repulsion can split the energy bands into two subbands, the so-called the upper and lower Hubbard bands (UHB and LHB) and cause the insulating behavior at half-filling. This can be easily found by
considering the band structure in the atomic limit, i.e. the bandwidth $W = 4t$ vanishes. In this limit, the system reduces to an array of independent atoms with on-site Coulomb repulsion, whose single-site spectrum consists of $E_0 = 0$ for empty state $|0\rangle$, $E_1 = \epsilon_{at}$ for two singly-occupied state $|\sigma\rangle$ with $\sigma = \uparrow, \downarrow$, and $E_2 = 2\epsilon_{at} + U$ for doubly-occupied state $|\uparrow\downarrow\rangle$. It means that the second electron (refer to Fig.1.10(a)) added to the singly-occupied site can cost additional energy $U$. In general, the band structure of the system can be schematically represented as shown in Fig.1.10(b-d), where the UHB and LHB are symmetric in the presence of particle-hole symmetry. The center of these two bands are separated by the on-site repulsion $U$, so if the bandwidth is large enough, they can overlap, leading to the metallic phase; otherwise, there is a charge gap $\Delta_c$ between the edges of the subbands. In other words, the system can shift from insulating phase to metallic phase as the ratio $\frac{U}{t}$ decreases.

Figure 1.10: Schematic band structure of one-band Hubbard model in the “atomic” limit a) and general case b)-d). In b)-d), the black band represents the LHB and the white one denotes the UHB. There is a critical value of $U_c$, above which the system becomes insulating.

Symmetries: The Hubbard model can support many symmetries, like the translational symmetry or the symmetry under spin flips. For one-dimensional Hubbard model, there are some additional symmetries that depend on the ratio $\frac{U}{t}$ and closely relate to the solvability of the model. Here we concentrate on the formal symmetries, that are of three kinds: spatial symmetries related to the lattice, symmetries connected to the spin and particle-hole symmetries.
**Spin-rotation symmetry SU(2)**: In the absence of magnetic field, the system is invariant under spin rotation

\[ c'_{i\sigma} = \sum_{\sigma'} U_{\sigma\sigma'} c_{i\sigma'} \]

where \( U \in SU(2) \), since

\[ H_0 = -t \sum_{<i,j>\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.}) \rightarrow H'_0 = -t \sum_{<i,j>\sigma,\sigma'\sigma''} (c^\dagger_{i,\sigma''}(U^\dagger_{\sigma''\sigma} U_{\sigma\sigma'}) c_{j,\sigma'} + \text{h.c.}) = H_0 \]

and the interaction term can be rewritten as

\[ H_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow} = -\frac{2U}{3} \sum_i (\vec{S}_i)^2 + \frac{NU}{2} \]

**Particle-hole symmetry**: This discrete symmetry is related to the underlying lattice structure of the Hubbard model. Under the particle-hole transformation

\[ c^\dagger_{i\sigma} = (-1)^i c_{i\sigma} \]

the local density operator \( n_{i\sigma} \) changes as

\[ n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} \rightarrow n'_{i\sigma} = c_{i\sigma} c^\dagger_{i\sigma} = 1 - c^\dagger_{i\sigma} c_{i\sigma} = 1 - n_{i\sigma} \]

where the electron density is mapped onto the hole density, so the interaction term can be easily written in an invariant form

\[ H_{\text{int}} = U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \rightarrow H'_{\text{int}} = U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \]

This new form differs from the original one only by a trivial shift in the chemical potential and an overall additive constants to the energy. Accordingly, the
kinetic term changes as

\[ H_0 = -t \sum_{<i,j>,\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) \rightarrow H_0' = t \sum_{<i,j>,\sigma} (-1)^{i+j}(c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) \]

For the bipartite lattices, such as square or honeycomb lattice, \((-1)^{i+j} = -1\) is guaranteed, so \(H_0' = H_0\). If the chemical potential is taken into account, we obtain the grand-canonical potential, also referred to as the Hubbard model, which becomes

\[ H = -t \sum_{<i,j>,\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) + U \sum_i (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2}) - \mu \sum_i (n_{i,\uparrow} + n_{i,\downarrow}) \]

where the last term preserves the particle-hole symmetry if the sign of the chemical potential is reversed, i.e. \(\mu\) is replaced by \(-\mu\). Thus, it is enough to study the system with either electron or hole doping.

**From repulsion to attractive** : There is an additional particle-hole transformation

\[ c_{i,\uparrow} \rightarrow c_{i,\uparrow} \quad c_{i,\downarrow} \rightarrow (-1)^i c_{i,\downarrow} \]

which preserves the kinetic energy in the bipartite lattice, but changes \(U \rightarrow -U\), since

\[ (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2}) \rightarrow -(n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2}) \]

So it can map the attractive Hubbard model to the repulsive one. More interestingly, it maps the charge sector of the Hubbard model on the spin sector and vice versa, since \(\mu \leftrightarrow h\),

\[ n_{i,\uparrow} + n_{i,\downarrow} \rightarrow n_{i,\uparrow} - n_{i,\downarrow} + 1 \quad n_{i,\uparrow} - n_{i,\downarrow} \rightarrow n_{i,\uparrow} + n_{i,\downarrow} - 1 \]
At half-filling $\mu = 0$ and in the absence of magnetic field, this transformation just change $U \rightarrow -U$. Note that this symmetry at half-filling can be promoted to $SO(4) = SU(2) \times SU(2)$ if it combines with spin-rotation symmetry and supports bosonic representation. This symmetry is quite useful for the classification of the low-lying states in the 1D Hubbard model.

**Hubbard chain** : The physics captured by the Hubbard model depends on the underlying lattice structures. The simplest case is the one-dimensional Hubbard model—Hubbard chain, which can be described by the following Hamiltonian

$$H = -t \sum_{i=1}^{L} (c_{i\sigma}^\dagger c_{i+1\sigma} + H.c.) + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow}$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron of spin $\sigma$ on the $i$th site along a chain of length $L$, $n_{i}$ represents the local density operator. As a one-dimensional model, it has been exactly solved by Lieb and Wu [29] using the Bethe ansatz. This is an important benchmark showing that for all $U/t$, the solution at $T = 0$ is a metal with Fermi surface the same as for $U = 0$, away from half filling. In fact, its low energy excitations can be understood in the context of Luttinger liquid (LL) theory. At half-filling $n_{\uparrow} = n_{\downarrow} = \frac{1}{2}$, such systems have odd number of valence electrons per unit cell and yet become *Mott insulators*, in contradiction with predictions of band theory, unless the interaction $U$ vanishes. Physically, this charge gap is open due to the unique $4k_F$-Umklapp scattering term present for half filling, but spin gap remains vanishing. In spite of such success, it is not known how to extend the solution to higher dimensions, including the 2-dimensional Hubbard model, which are relevant to the high-$T_c$ cuprate superconductors. So the study of higher-dimensional Hubbard models, especially two-dimensional Hubbard model requires approximate/numerical methods. The 1-dimensional Hubbard chain itself can be a testing ground for the validity of various new methods in studying strongly correlated systems.
In the following, we briefly review the spectrum of low-lying excitations of the 1D Hubbard model (from [3]). In addition to the conventional electron-hole pairs, it can create charge excitations by adding or removing particles from the ground state, and spin excitations by reversing the spin of an electron. We will consider the half-filled and away from half-filled case separately.

**Half-filled band**: For the half-filled band, the elementary excitations include spinons and holons.

**Charge excitations—holons/antiholons**: These are gapped and spinless excitations carrying charge $-e$ and $e$, which correspond to antiholon and holon respectively. Their dispersions have the same gap which can increase with $u = V_{4t}$ but reach minimum at different momentum (shown in Fig. 1.11(a) and (b)). Note that both holon and antiholon momenta cover the entire Brillouin zone.

**Spin excitations—Spinons**: These are gapless but charge-neutral excitations carrying spin $\pm \frac{1}{2}$, called spinons. Their dispersions contain gapless modes at $P_s = 0, \pi$ (shown in Fig. 1.11 (c)). Note that their momentum only covers half the Brillouin zone.

Figure 1.11: Dispersions of the elementary holon (a), antiholon (b) and spinon (c) excitations for $u=0.25, 0.75$ and $u=2.5$. From [3]. Note that the energy of holon has a minimum at $P_h = -\frac{\pi}{2}$ and the holon energy at $P_h = \frac{\pi}{2}$. For spinons, the energy have two minima at $P_s = 0$ and $\pi$. 

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From the dispersions, we can easily find that the “bandwidth” of charge excitation is independent of $U$ but the “bandwidth” for spinons is reduced as $U$ increases. Quantitatively, we obtain

$$W_{\tilde{h},\tilde{h}} = 4t \quad W_s \sim \frac{8t^2}{U} = 2J$$

Additionally, if we compare the slopes of holon and spinon dispersions near their minima, we can obtain that they have different velocities, as indicated by the spin-charge separation.

In half-filled case, there are no excitations involving only one spinon or one (anti)holon. Any low-lying states can be thought of as a scattering state of an even number of these elementary excitations constrained by some selection rules. Technically, they furnish the irreducible representation of $SO(4) = SU(2) \times SU(2)$. In the following, we just consider the two-particle sector involving two elementary excitations. In this sector, group theory tells us the classification of excitations as follows

$$(0, \frac{1}{2}) \otimes (0, \frac{1}{2}) = (0, 1) \oplus (0, 0)_c \quad (\frac{1}{2}, 0) \otimes (\frac{1}{2}, 0) = (1, 0) \oplus (0, 0)_s \quad (0, \frac{1}{2}) \otimes (\frac{1}{2}, 0) = (\frac{1}{2}, \frac{1}{2})$$

corresponding to two (anti)holons, two spinons and spinon-(anti)holon excitations:

**Charge Triplet/Singlet excitation** : They are gapped excitations, corresponding to the $(1,0)$ and $(0,0)_c$ representation of $SO(4)$. As compound objects, their dispersions are continuum as shown in Fig.1.12(a) due to their underdetermined relative momenta. As expected, its bandwidth is 4 unit of energy.

**Spin Triplet/Singlet excitation** : They are gapless excitations, corresponding to the $(0,1)$ and $(0,0)_s$ representation of $SO(4)$. The spin triplet excitations (as shown in Fig.1.12(b)) are very similar to the spin triplet Heisenberg spin-$\frac{1}{2}$ antiferromagnet, and can be probed by inelastic Neutron Scattering Experiments.
Spin-Charge scattering states: They are gapped two-particle excitation, corresponding to the \((\frac{1}{2}, \frac{1}{2})\) representation of \(SO(4)\). This type of excitation is of particular importance for photoemission experiments like ARPES, where an electron is removed and the system gets excited into a state with quantum numbers \((-\frac{1}{2}, \pm \frac{1}{2})\).

\[\text{Figure 1.12: Upper and lower boundaries of the scattering continuum for the charge singlet excitation, spin triplet excitation, spin-charge scattering state, respectively.}\]

Less than half-filled band: In contrast to the half-filled case, the ground state of the system with less than half-filled band \(0 < n < 1\) becomes metallic, since there is no charge gap as mentioned above. In this case, there are three different kinds of elementary excitations: gapless (anti)holons, gapless spinons and gapped excitations. As in the half-filled case, neither single spinon nor (anti)holon presents in physical spectrum, which includes gapless excitations formed elementary excitations pairs and single-particle excitations involving the so-called \(k - \Lambda\) strings. In this case, the physical excitations can be classified according to the quantum number of an electron. In the following, we just list some of them as examples. More details can refer to [3]

Charged neutral excitations: This sector involves particle-hole excitations, in addition to spin triplet and spin singlet excitations. Particle-hole excitations are gapless physical excitations with spin and zero charge, and their low-energy modes occurs at momenta 0 and \(\pm 2\pi n \text{ mod } 2\pi\).
**Charged excitation**: This sector involve “Antiholon-Spinon”, “Holon-Spinon” excitations and $k - \Lambda$ string of length 2. The “Antiholon-Spinon” excitation has the quantum numbers of an electron, i.e. spin $\pm \frac{1}{2}$ and charge $-e$ with respect to the ground state, corresponding to the state with one electron added to the ground state. Similarly, the “Holon-Spinon” excitation corresponds to the state with one electron removed from the ground state. The last excitation is the simplest excitation involving a $k - \Lambda$-string. It has the same quantum numbers as the ground state. Physically, these string states are bound state but with energy higher than that of a scattering state of two electron. This strange result makes sense because the bound-state property is just a lattice effect and does not survive in a continuum limit.

**Hubbard ladder**: Hubbard ladders contain multiple Hubbard chains that get coupled together and play an vital role in understanding the physics of crossover from 1D to 2D Hubbard model. The half-filled Hubbard ladder with even legs behaves as an insulating spin-gapped system, exhibiting a crossover from a spin-liquid to a band-insulator as a function of the interchain hopping $t_\perp$. In the strong $t_\perp$ limit, the transverse exchange $J_\perp$ is large, so the spins on a rung are locked into a singlet state, called *rung singlet*. On the other hand, doped-Hubbard ladder has been studied to probe the pairing mechanism of holes: It has been confirmed that spin and charge tend to get paired forming bound states called polarons. Meanwhile, holes can gain energy by pairing, as shown in Fig.1.13. This can be understood as follows: In the large $U$ limit at half-filling, it is equivalent to two-leg spin ladder. If the super-exchange coupling along the rung $J_\perp$ is much larger than that along the leg $J_\parallel$, the system becomes an array of rung-singlets with large spin gap. After doping, the singlet bonds may break leaving out unpaired spins, or rung holes may get paired, yielding an additional rung-singlet. This is the process of competition between kinetic and magnetic energies. When pairing correlations dominate, hole pairing wins with binding energy $\Delta_{\text{binding}} \sim J_\perp$. But spin gap is very robust and survives in both cases.
**Infinite dimensional Hubbard model**: In infinite-dimensional case, the behavior of the model does not necessarily become a mean-field like but remains tractable under some conditions [31]. It gives a striking result that provides us a understanding of the Mott transition between a paramagnetic metal and a correlated insulator. More importantly, it triggers the invention of dynamic mean field theory (DMFT) [32], which is known as one of the most important numerical tools for solving strongly correlated systems.

**$U \gg t$ regime: $t - J$ model and Heisenberg models**  In the strong coupling limit, i.e. $U$ is quite large, double occupancy is not favorable, so one can project out them from the full Hilbert space of the Hubbard model, and map the problem onto an effective low energy theory described by the so-called $t - J$ model

$$H = -t \sum_{i=1}^{L} (\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{i+1\sigma} + H.c.) + J \sum_{i=1}^{L} (\vec{S}_{i} \cdot \vec{S}_{i+1} - \frac{1}{4} n_{i} n_{i+1})$$

where the tilde sign indicates the constraint forbidding double-occupancy, $\vec{S}_{i}$ is the spin operator, and $J = \frac{4t^{2}}{U}$ essentially parameterizes the exchange interaction between spins. (Note that a quantitative agreement of one-particle spectra between the Hubbard and $t - J$ models cannot be reached unless more corrections to the $t - J$ models, such as three-site terms, and wavefunction correlations, are included.)

Due to the constraint, the projected fermionic operators $\tilde{c}_{i\sigma}$ and $\tilde{c}_{i\sigma}^{\dagger}$ don’t follow the ordinary anticommutation relation, which poses a problem as there is no conventional occupation-number representation. This can result in a non-Fermi liquid. In
addition, the kinetic energy ($\sim t_{ij}$) and the exchange ($\sim J$) can be comparable close to the half filling and result in transition or instability.

**t-J chain**: Compared to the one-dimensional Hubbard model, the $t - J$ model possesses a much richer phase diagram if the so-called unphysical regime ($J \geq t$) is taken into account. Using the density matrix renormalization group (DMRG), it has been found that 1D $t - J$ model supports 4 different phases ([4]): a metallic phase, a glass superconducting region, a singlet-superconducting phase with spin gap, and phase separation (shown in Fig.1.14(a)).

![Figure 1.14](image)

**Figure 1.14**: a). Phase diagram of the 1D $t - J$ model from DMRG for densities $0.1 \leq n \leq 0.9$ and in the range $0 < J \leq 4$, where we set $t = 1$ and $n = \frac{N}{L}$ is the electronic density. There are four phases present: a metallic phase (M), a gapless superconducting (SC) phase, a singlet-superconducting phase with spin gap (SG+SS), and phase separation (PS). from [4]. b). Cartoon describing the formation of hole pairs (see context).

For smaller $J < 2$, the system remains metallic phase for all densities $n$. This corresponds to the repulsive Luttinger liquid phase, meaning that both spin and charge gaps are closed. Interestingly, for intermediate $J \sim 2 - 3$, the realization of phase of the chain depends on the electronic filling, meaning that we can create hole pairing by tunneling the parameter $n$. Meanwhile, the spin gap can be opened as well. For large $J/t$, the phase separation phase, where the system separates into a hole-rich and an electron-rich part forming an antiferromagnetic island, takes place. This can easily be understood (see Fig.1.14(b)): Introducing one hole to the chain will break two anti-ferromagnetic bonds around it. So for holes far from each other,
the system loses 4 antiferromagnetic bonds. However, if these holes are put close together, only 3 bonds are broken. Thus, if $J/t$ is large, the $t-J$ chain has a strong tendency to phase separation.

**Heisenberg model** At half-filling, the $t-J$ model can further reduce to the Heisenberg model

$$H = J \sum_{i,\delta} \vec{S}_i \cdot \vec{S}_{i+\delta}$$

, where the hopping of electrons is completely forbidden due to the double occupancy constraint. The Heisenberg model is also a paradigmatic model in condensed matter physics: It is relatively simple and can describe real materials, such as low-dimensional quantum magnets. Its various generalizations, which may take into account the interactions beyond nearest neighbors, anisotropic couplings, different underlying lattice structures and so on, have been widely studied.

**Heisenberg chain** : The one-dimensional Heisenberg model is a prototypical integrable system, which can be solved exactly by the Bethe Ansatz, and can also be studied using bosonization techniques and conformal field theory. For positive $J$, its ground state doesn’t spontaneously break any symmetries, as indicated by the Mermin-Wagner theorem. Physically, this is due to the quantum fluctuations in lower dimensional system: Spin fluctuations in one dimension are so strong that it can kill any long-range order. The nature of correlation depends on the spin of the components: If the spin is integer, then only short-range order is present, i.e. the spin-spin correlation decays exponentially with the inter-spin distance due to the Haldane gap. For half-integer spins, the systems exhibit quasi-long range order, meaning that the spin-spin correlation decays algebraically.
1.2.2 Application of the Hubbard model to HTSC

As mentioned above, the essential physics of high-$T_c$ cuprates superconductor can be captured by the behavior of the electrons/holes in the $CuO_2$ planes, so as a first approximation we can construct effective Hamiltonians to describe this $CuO_2$ plane, in which each unit cell contains one copper and two oxygen ions. Although this approximation has radically reduce the number of effective degrees of freedom, describing the $CuO_2$ unit cell is not easy since it contains so many orbitals and electrons. To build the model, we need to identify the active orbital that participates the electronic and magnetic processes.

**Lifting the degeneracy**  : In the undoped parent compound, the copper ion has the electronic configuration $3d^9$ while the oxygens receive two electrons (one from the copper, the other being provided by the charge reservoir). Thus all three 2p-orbitals of the oxygens are filled and so are the four of the five-fold 3d orbitals of the copper. To determine the active orbital of Cu, we need to take into account the orbital degeneracy of 3d orbitals in Cu ions lifted by crystal fields (shown in Fig.1.15(a)). Within the $CuO_2$, the partially filled orbital $d_{x^2-y^2}$ can hybridize with the 2p orbital of oxygen ions and result in the hybridized orbitals. From the figure, we can see that the band with the highest energy results from the hybridization of the Cu $d_{x^2-y^2}$ and one of the O2p$_\sigma$-orbitals, referred to as the upper antibonding band. It is convenient to characterize the undoped Cuprate compounds in terms of holes rather than electrons, e.g. the ‘vacuum’ for the holes is given by the fully electron-filled configuration and the lowest-energy state for the holes is the highest energy state for the electrons, i.e. the antibonding $d_{x^2-y^2}$ band, meaning that the energy level in Fig.1.15(b) needs to be turned upside-down in the hole-picture.

**Three-band description—charge transfer insulator**  : To characterize the strong correlations in cuprates, we need to take into account the on-site Coulomb repulsions $U_d$ and $U_p$ for the Cu and the O ions, respectively. As a multi-orbital
Figure 1.15: a). Crystal-field splitting of 3d orbitals of Cu$^{2+}$: In the ideal case, each Cu$^{2+}$ is surrounded by a regular octahedron of oxygen ions O$_6$, with all Cu – O – Cu angle being 180°. As a result, the 3d orbitals are partially lifted and get split into a lower triplet (so-called $t_{2g}$) levels involving $d_{xy}$, $d_{yz}$, $d_{xz}$ and an upper doublet $e_g$ including $d_{3z^2-r^2}$ and $d_{x^2-y^2}$. The resulting system is double degenerate and is unstable due to the Jahn-Teller theorem, which predicts an unavoidable structural transition further lowering the symmetry of the crystal and lifting the remaining orbital degeneracy. For instance, the energy of $d_{x^2-y^2}$ can be larger than that of $d_{3z^2-r^2}$. b). Level splitting between Cu$^{2+}$ and O$^{2-}$ ions due to the orbital hybridization. The numbers in parentheses indicate the occupations of the different levels in the undoped compound. From [5]

model, there is an additional energy gap $\Delta = \epsilon_p - \epsilon_d$ corresponding to the charge transfer between the copper and the oxygens. If the $p$ orbital falls in between the Hubbard subbands (shown in Fig.1.16(b)), which requires $U > \Delta > 0$, the system is a charge transfer insulator, meaning that the holes are tightly bound with the Cu at half-filling. When additional holes are doped into the CuO$_2$, they are observed to prefer to go onto the highest O-level, which is consistent with the fact that the Coulomb repulsion between holes strongly disfavors doubly-occany of the Cu $d_{x^2-y^2}$-orbital.

Putting all together, Emery [33] proposed a three-band model which takes into account the on-site Coulomb repulsion and three orbitals Cu3$d$, O2$p_x$ and O2$p_y$, 27
Figure 1.16: Schematic energy band diagrams for Mott insulator (MI), Charge transfer insulator (CTI) and their doped cases without considering the hybridization effect: a). In MI, the oxygen orbital is lower in energy than the LHB; b). In CTI, the oxygen orbital falls in between LHB and UHB. c). Hole doping moves the Fermi level into the lower Hubbard band, while electron-doping shifts it into the upper Hubbard band. d). Hole doping moves the Fermi level into the oxygen p band, while electron-doping moves it into the upper Hubbard band. From [6].

Given by

\[
H = \Delta \sum_{\sigma} p_{i\sigma}^d p_{i\sigma} - t_{pd} \sum_{\langle ij \rangle < \sigma} (d_{i\sigma}^d P_{j\sigma} + p_{j\sigma}^d d_{i\sigma}) - t_{pp} \sum_{\langle ij \rangle > \sigma} (p_{i\sigma}^d P_{j\sigma} + p_{j\sigma}^d p_{i\sigma}) 
+ U_d \sum_i n_{i\uparrow}^d n_{i\downarrow}^d + U_p \sum_i n_{i\uparrow}^p n_{i\downarrow}^p + V_{pd} \sum_{\langle ij \rangle} n_{i\uparrow}^d n_{j\uparrow}^p + V_{pp} \sum_{\langle ij \rangle} n_{i\uparrow}^p n_{j\uparrow}^p.
\]

Here \( \Delta = \epsilon_p - \epsilon_d \) is the energy difference between having a hole on an O site versus a Cu site, \( t_{pp} \) and \( t_{pd} \) are one-hole hopping matrix elements between near-neighbor O sites and near-neighbor Cu and O sites, respectively. \( U_d \) and \( U_p \) are the onsite Cu and O Coulomb interactions and \( V_{pd} \) and \( V_{pp} \) are the near-neighbor Cu-O and O-O Coulomb interactions, respectively. Note that \( U_d \) usually dominates over other two interactions, i.e. \( U_d \gg U_p > U_{pd} \).

Qualitatively, we can find one of the key features in doping the charge transfer insulator (CTI) (shown in Fig.1.16(d)): it breaks the particle-hole symmetry, meaning that its phase diagram is asymmetric about the doping \( x = 0 \), which is consistent with experiments (see Fig.1.7).
Toward a one-band model—Zhange-Rice singlet: As a minimum model for HTSC, the 3-band Hubbard model can capture essential physics but is very difficult to study since it still contains too many degrees of freedom. This makes people pursue simpler but still effective descriptions for cuprates, in the sense that it arises as a strong-coupling limit from the three-band Hubbard model but involves fewer degrees of freedom. Most importantly, it should address the AFM and SC phases observed in the material of interest, which constraints the energy scale of the model. After careful analysis [34], Zhange and Rice made great progress along this direction and proposed the idea that the hole confined to the copper at half-filling can form singlet, called “Zhang-Rice singlet”, with dopant-holes on the oxygens around it (see in Fig.1.17), since their exchange interaction is so strong that its triplet excitations is ignorable. In other words, the Zhang-Rice singlet plays the role as an inert object that can hop with effective hopping \( t_{eff} \). As a result, the original lattice composed of \( CuO_2 \) reduces to a new lattice made only out of Cu atoms, i.e. the original unit cell containing one copper and two oxygens reduces to a single site and two \( p \) orbitals of oxygen ions can be effectively removed from the model. With this knowledge, the effective model for the singlet can be written as an effective \( t - J \) model. But in practice, theorists study the more generic 2D one-band Hubbard model, which is supposed to mimic low-energy spectrum near the half-filling using a set of effective parameters. However, we should keep in mind that the one-band Hubbard model preserves particle-hole symmetry (see Fig.1.16(c)) unless some other terms like the next-nearest neighboring hopping are included explicitly.

1.3 Angle-resolved Photoemission Spectroscopy (ARPES)

Angle-resolved photoemission spectroscopy (ARPES) is an advanced experimental technique to directly probe the single-particle excitation spectrum \( E(k) \) based on the photoelectric effect with a high precision, i.e. it can provide the density of single-particle electronic excitations in the reciprocal lattice of the solid under
study. Compared to its precursor, photoemission spectroscopy (PES), which studies photoemission of electrons from a sample achieved usually by illumination with soft X-rays, ARPES uses ultraviolet light to generate photoemission and can give detailed information on the direction, speed and scattering process of valence electrons in the solids, solid surfaces and interfaces. It means information on both the energy and momentum of an electron can be gained, resulting in electronic band dispersion and Fermi surface.

1.3.1 From PES to ARPES

Since 1905, the “photoelectric effect” has been understood by Einstein with the aid of quantum idea (as shown in Fig.1.18(a)): An electron inside a sample might absorb an incoming photon and get excited. If the energy $h\nu$ of the incoming photon is high enough, the electron can escape from the material, becoming a photoelectron with a maximum kinetic energy of $E_{kin}^{max} = \hbar \omega - \phi$, where $\phi$, representing the gap between the vacuum energy level and the Fermi energy level, is a measure of the potential barrier at the surface of the material that prevents the valence electrons from escaping and is typically 4-5 eV in metals. Note that the energy of incoming photons should be appropriate: If it is too low, the excited electron cannot acquire enough energy to overcome the potential barrier at the surface and fail to escape.
the material. If it is too high, more involved phenomena, like Thomson scattering, Compton scattering or even pair production, can complicate the situation.

Figure 1.18: Cartoon describing the photoelectric effect on a sample in panel a). Panel b) shows the relation between the energy level in a solid and the electron energy distribution produced by photons of energy $\hbar \omega$ from [7].

To understand the experimental spectrum of PES in solids, it is more appropriate to consider the relation between the energy-level diagram and the energy distribution of photoelectron (sketched in Fig.1.18(b)) (Note that the energy-level diagram holds in a one-particle picture). In solid samples, electrons can occupy core levels and valence bands. For metals, the Fermi energy $E_F$ sits at the top of the valence band and has a gap $\phi$ from the vacuum level. If the valence electrons are ejected, the associated kinetic energy is the same as above. But if the photoabsorption occurs in a core level with binding energy $|E_B| = E - E_F$, the emitted electrons can be detected with the maximum kinetic energy

$$E_{\text{kin}}^{\text{max}} = \hbar \omega - \phi - |E_B|$$

in the vacuum. Typically, the energy distribution of the emitted electrons is plotted as a function of the binding energy $E_B$, rather than the kinetic energy $E_{\text{kin}}$, with $E_F$ taken as the zero. For instance, in the left panel of Fig.1.19, we can clearly identify both valence band and core levels and read off the binding energies for both
4f doublets $|E_B(4f_{7/2})| \approx 84.0\text{eV}$ and $|E_B(4f_{5/2})| \approx 87.7\text{eV}$ below $E_F$. In the right panel, the shape of the Fermi distribution at finite temperature can be determined. As expected, PE spectroscopy can provide us the electron-energy distribution in a material but the information about electronic momentum is totally lost. The urge to acquire the electronic momentum distribution gives the impetus on the development of the ARPES techniques.

The advent of ARPES is entirely due to several important advancements including the improvement of the energy resolution of the light source, such as synchrotron radiation and laser sources, and of the detector. This new technique can measure both the kinetic energy and angular distribution of the electrons emitted from a sample impinged with sufficiently high-energy photons. Based on this set of information, one can gain the knowledge on both the energy and momentum of the electrons inside a material, which is of vital importance in elucidating the interplay of charge, spin, lattice and even orbital degrees of freedom in solids. So it can provide us with rather deep insights into the low-lying single-particle excitations of the solid, in particular whenever many-body physics becomes important.

**Figure 1.19:** Illustrations of PES spectrum: a). XPS spectrum ($\hbar \omega = 1487\text{eV}$ of polycrystalline Au for $0 \leq E_B \leq 100\text{eV}$). Here both the 5$d$ valence band and the $4f_{7/2}$ doublet are clearly seen. b). Energy distribution around $E_F$ in an UPS spectrum ($\hbar \omega = 21.2\text{eV}$) from a polycrystalline Ag sample. The Fermi distribution at finite temperature can be clearly identified. Both are from [7]
1.3.2 What ARPES measures

The geometry of an ARPES experiment is sketched in Fig. 1.20: An electron energy analyzer is adopted to collect the photoelectrons in a finite acceptance angle and measure their kinetic energies $E_{kin}$ for a given emission direction. In terms of the polar ($\theta$) and azimuthal ($\varphi$) angles, one can obtain the three components of momentum of emitted electrons:

\[
\begin{align*}
    k_x &= \frac{\sqrt{2mE_{kin}}}{\hbar} \sin \theta \cos \varphi \\
    k_y &= \frac{\sqrt{2mE_{kin}}}{\hbar} \sin \theta \sin \varphi \\
    k_z &= \frac{\sqrt{2mE_{kin}}}{\hbar} \cos \theta
\end{align*}
\]

where $k_z$ gives the component of momentum perpendicular to the sample surface and $\mathbf{k}_\perp = k_x \hat{x} + k_y \hat{y}$ corresponds to the perpendicular component. The motivation of ARPES is to deduce the relation between binding energy $E_B$ and momentum $\mathbf{k}_i$ for the electrons moving inside the solid, starting from the function $E_{kin}(\mathbf{k})$ measured in vacuum. This can be done by exploiting the energy and momentum conservation laws

\[
E_f - E_i = \hbar \omega \\
\mathbf{k}_f - \mathbf{k}_i = \mathbf{p}
\]
where $p$ is the momentum of the incoming photon, the index $i$ and $f$ denote the quantities before and after the optical transition process. Due to the presence of interface between the sample and vacuum, which breaks the translational symmetry perpendicular to the sample surface, the perpendicular component of crystal momentum is not conserved and the momentum $k_\parallel$ equals the parallel component of the crystal momentum of electron inside the solid in the extended zone scheme, meaning that

$$k_\parallel = k_{f\parallel} + G$$

where $G$ denotes the reciprocal lattice vector. Hence, without additional information, the crystal momentum cannot be determined completely. In the case of lower-dimensional systems, the uncertainty in $k_\perp$ becomes irrelevant, since the electronic dispersion is almost exclusively determined by $k_\parallel$. In a PES experiment, the angle- or momentum-resolved energy distribution curves (EDCs) are measured and can be used to determine the dispersion of electronic excitations by tracing the energy positions of marked features as is illustrated in Fig.1.21(a) and (b).

![Figure 1.21: Angle-resolved photoelectron spectroscopy: a). Momentum-resolved energy distribution curves (EDC) for a non-interacting electron system with a single band, crossing the Fermi energy $E_F$. b). EDC for an interacting Fermi liquid from [8]. The corresponding ground-state momentum distribution function $n(k)$ at zero temperature in both cases are also shown. c). The PES spectrum of hydrogen in the gas phase and the hypothetical spectrum for solid hydrogen (dashed line) from [8]. These spikes correspond to electronic-vibrational eigenstates, the excitation of internal degrees of freedom of hydrogen molecules.](image)
1.3.3 Three-step model description of the photoemission process

The photoemission process in a solid is rather complicated and its full calculation still represents a challenging task. In the following, we will consider a rather simple model, the so-called three-step model (shown in Fig.1.22), that is used to describe the photoemission process. This model given by Berglund and Spicer [35] is phenomenological, but it proves to be rather successful. In this model, the photoemission process is artificially broken up into three independent steps:

1. Optical excitation of the electron in the bulk. This step is described by the probability for the optical transition, which contains all of the information about the intrinsic electronic structure of the material.

2. Travel of the excited electron to the surface. This step is characterized by the scattering probability for the propagating electron, which can be effectively parameterized in terms of an effective mean free path, proportional to
the probability that the excited electron will reach the surface without scattering. In this step, the inelastic scattering processes, which determine the surface sensitivity of photoemission, give rise to a continuous background in the spectra, which is usually ignored or subtracted.

3. Escape of the photoelectron into vacuum. This step can be depicted by the transmission probability through the surface potential barrier, which depends on the energy of the excited electron and the material work function $\phi$.

It provides a rather comprehensible picture of the photoemission process and simplifies the calculation of the total photoemission intensity, which is then given by the product of three independent terms: the total probability for the optical transition, the scattering probability for the traveling electrons and the transition probability for the traveling electrons. But it completely ignores self-energy corrections to the initial and final state, which give rise to damping processes and energy shift, since it assumes both the initial and final states are Bloch states with an infinite lifetime. This assumption does not allow for transitions into evanescent states and fails to allow us to calculate photoemission spectra from surface states. These limitations can be corrected by a more rigorous approach, the so-called \textit{one-step model} in which photon absorption, electron removal, and electron detection are treated as a single coherent process and bulk, surface and vacuum are included in the Hamiltonian, which can give not just bulk states under study, but also surface and evanescent states, as well as surface resonances. But the model is more complicated compared to the three-step model.

1.3.4 Understanding the ARPES spectra: Correlations

In real material, the pervasive many-body interactions can involve various degrees of freedom and yield all possible excitations. In fact, even in a much simpler case like gaseous hydrogen (as shown in Fig.1.21(c)), the creation of a photoelectron
is simultaneously accompanied by the excitation of oscillations in $H_2$ molecules, which manifests itself as a series of satellite lines, besides the sharp line at about 6.8 eV corresponding to the excitations from the ground state. Physically, these satellites characterize the dynamics of electron-proton couplings. Furthermore, if the spectrum is broadened, these spikes get overlapped and form a more smooth dispersion like the hypothetical spectrum (dashed line) for solid Hydrogen, which can serve as a paradigm of PES spectrum for interaction solids. In more complex systems like a conventional metal, excitations could be either electron-hole pairs, or collective excitations \textit{plasmons} corresponding to the relative oscillation of the electrons with respect to the system of lattice ions. The ARPES can provide unique insight into the rich physics induced by various possible excitations of the systems and their many-body interactions.

To understand ARPES and especially analyze the experimental data quantitatively, a theoretical description of photoemission that bridges the gap between experiments and microscopic models is necessary. For simplicity, we adopt the three-step model and only focus on the photo-excitation step: The Fermi’s Golden Rule gives the expression of the photocurrent $I$ resulted from the photoexcitation

$$I_\kappa(\hbar \omega) = \frac{2\pi}{\hbar} \sum_n |\langle \Psi_{\kappa,n}(N)|H_{\text{int}}|\Psi_0(N)\rangle|^2 \delta(E_{\kappa,n}(N) - E_0(N) - \hbar \omega)$$

where $|\Psi_0(N)\rangle = |N, 0\rangle$ represents the N-electron ground state with energy $E_i = E_{N,0}$, $|\Psi_{\kappa,n}(N)\rangle = |N - 1, n; \kappa\rangle$ denotes all possible final states describing a system with $N - 1$ electrons in the solid and one photoelectron with quantum number $\kappa$. Here the index $n$ denotes a complete set of quantum numbers defining all possible excitations in the final state, and $H_{\text{int}}$ describes the interaction of the photon field with a single electron within first-order perturbation theory. Schematically, the interacting Hamiltonian can be parameterized by

$$H_{\text{int}} = \sum_i M_{ij} c_{n_j}^\dagger c_k$$

37
where $M_{if}$ denotes the one-particle matrix elements, then the photocurrent becomes

$$I_\kappa(\hbar\omega) = \frac{2\pi}{\hbar} \left| \sum_i |M_{if}|^2 \sum_n |\langle N-1, n; \kappa|c_{n,f}^\dagger c_{\kappa,i}|N, 0\rangle| \right|^2 \delta(E_{\kappa,n}(N) - E_0(N) - \hbar\omega)$$

To go further, two assumptions are usually taken to simplify the problem: the independent-particle picture and the sudden assumption.

**The independent-particle picture**: The photoelectron is treated as a free electron with wavevector $\kappa = k_f$ and energy $\epsilon_{k_f}$, meaning that the band dispersion of photoelectron is replaced by a simple quadratic dispersion. So the final state becomes $|N-1; n, \kappa\rangle \approx |N-1, n; k_f\rangle$.

**The sudden approximation**: The escaping photoelectron is assumed to decouple from remaining system immediately after photoexcitation, and relaxation processes during photoemission are neglected. So the final state is factorizable, i.e. it can be written as a product of the state of the photoelectron and the state of the remaining (N-1) particle system

$$|N-1, n; k_f\rangle \approx |N-1, n\rangle \otimes |k_f\rangle \equiv c_{k_f}^\dagger |N-1, n\rangle \otimes |0\rangle$$

, where $|N-1, n\rangle$ represents the $n$-th eigenstate of remaining N-1 electron system, and the final state energy becomes $E_{k_f,n}(N) = E_n(N-1) + \epsilon_{k_f}$. Note that this assumption is far from trivial because the system will relax during the photoemission process. It is valid only for high kinetic energy photoelectron limit. If the kinetic energy of photoelectrons is low, this assumption becomes inappopriate and alternative assumption like adiabatic limit can be assumed, since post-collisional interaction between the photoelectron and the remaining system cannot be simply ignored. For the cuprate high-temperature superconductors, the sudden approximation is valid even at photo energies as low as 20eV.
With these assumptions, the photocurrent can be further simplified as

\[ I_{kf}(\hbar \omega) = \frac{2\pi}{\hbar} \sum_i |M_{if}|^2 \sum_n |\langle N-1, n|c_{ki}|N,0 \rangle|^2 \delta(E_n(N-1) + \epsilon_{kf} - E_0(N) - \hbar \omega) \]

\[ = \frac{2\pi}{\hbar} \sum_i |M_{if}|^2 \sum_n |\langle N-1, n|c_{ki}|N,0 \rangle|^2 \delta(\epsilon + E_n(N-1) - E_0(N-1)) \]

\[ = \frac{2\pi}{\hbar} \sum_i |M_{if}|^2 A^<(k_i, \epsilon) \]

where we introduce \( \epsilon = \epsilon_{kf} - \hbar \omega - \mu \) with the chemical potential \( \mu = E_0(N) - E_0(N-1) \), and \( A^<(k_i, \epsilon) \) is the electron removal spectral function at \( T=0 \). If the one-particle matrix element \( M_{if} \) remains constant in the energy and \( k \)-range of interest, angle-resolved photoemission essentially measures the momentum-resolved spectral function \( A^<(k_i, \epsilon) \), which describes the probability to remove an electron from the system with momentum \( k \) and energy \( \epsilon \).

In the non-interacting case, the state \( c_{ki}|N,0 \rangle \) is an eigenstate of the \( (N-1) \)-particle system in some excited system, so it has a finite overlap with some particular final state and the ARPES displays as a delta peak at the band energy \( \epsilon_b^b \) as shown in Fig.1.21(a). In this case, the occupation number \( n_{\sigma}(k) \) displays a sudden drop from 1 to 0 at \( k = k_F \), which defines a sharp Fermi surface. In the interacting systems like Fermi liquids, the state \( c_{ki}|N,0 \rangle \) is no longer an eigenstate, meaning it has nonvanishing overlaps with many possible final states \( |N-1, n \rangle \). Therefore, the ARPES spectra will show a main line \( (n=k_i) \) and many satellites (other \( n \)) corresponding to a number of excited states created in the photoemission processes (as shown in Fig.1.21(b)).

To analyze the spectra quantitatively, we need the aid of many-body theory for the microscopic models, in which the spectral function can be parameterized by a
complex self-energy

\[
A^<(k, \epsilon) = -\frac{1}{\pi} \text{Im} G(k, \epsilon - i0^+)
= -\frac{1}{\pi} \text{Im} \frac{1}{\epsilon - \epsilon_k^0 - \Sigma(k, \epsilon)}
= -\frac{1}{\pi} \frac{\Sigma''(k, \epsilon)}{[\epsilon - \epsilon_k^0 - \Sigma'(k, \epsilon)]^2 + [\Sigma''(k, \epsilon)]^2}
\]

where the self-energy \( \Sigma(k, \epsilon) = \Sigma'(k, \epsilon) + i\Sigma''(k, \epsilon) \) characterizes the effect of interactions. The one-particle electronic excitations of the system is entirely determined by the analytic structure of the Green’s function \( G(k, \epsilon - i0^+) \) or equivalently of the spectral function \( A^<(k, \epsilon - i0^+) \).

In general, the exact calculation of \( \Sigma(k, \omega) \) is an extremely difficult task. Here we consider a particular case: Fermi liquids.

**Fermi liquid** : For Fermi liquids, the imaginary part of the self-energy only weakly varying with \( k \), the spectral function takes a Lorentzian shape whose finite width determines the finite lifetime of the electronic excitations inversely. The real part accounts for the renormalization of the electronic dispersion due to the interaction and is constrained by the presence of the Fermi surface via the renormalization condition. Formally, the Green’s function for Fermi liquid [(Pines1966)] can be written as

\[
G(k, \omega) = \frac{Z_k}{\omega - E_k + i\Gamma_k} + G_{\text{inch}}
\]

where \( Z_k = (1 - \frac{\partial \Sigma''}{\partial \omega})^{-1} \), \( E_k = Z_k(\epsilon_k + \Sigma') \) and \( \Gamma_k = Z_k|\Sigma''| \) represent the weight, renormalized dispersion and decay width of the quasi-particle, respectively. Here the self-energy and its derivatives are evaluated at \( \omega = E_k \). In addition, this description of Fermi liquid is valid only in the proximity to the Fermi surface. The last term \( G_{\text{inch}} \) contains information about the distribution of incoherent weights, characterizing electronic correlations.
1.3.5 Applications of ARPES experiments

As an advanced photo-excitation technique, ARPES has been widely applied to study electronic excitations of various interesting systems, including (quasi) 1D systems, cuprates, iron-based superconductors, topological insulators, and so on.

1.3.5.1 Spin-charge separation in Luttinger liquid

Experimental evidence for spin-charge separation effect has been sought for a long time. With the advent of ARPES, experimentalists looked forward to capturing the most direct evidence of spin-charge separation, the single quasiparticle peak splits into a spinon-holon two peak-like structure. At low energies, the dispersion should display double-cone structure, corresponding to the spinon and holon, respectively, since spinon and holon branches have different energy scales.

As a concrete example, ARPES data for $SrCuO_2$ are shown in Fig.1.23. From (a) in left panel, the 1D nature of $SrCuO_2$ is clear, since the intensity has almost no change as $k_\perp$ varies, meaning that intensity just depends on $k_\parallel$. Figure (c) provides much clear signal of spin-charge separation. From (a) in right panel, the dispersions of spinon and holon can fit the EDC, evidently elucidating the Luttinger liquid nature of the materials.

As another example, the ARPES spectrum of TTF-TCNQ is shown in Fig.1.24, where the experimental data (b) can be compared with the PES data of the doped 1D Hubbard model (a). Experimental data can be explained by the 1D Hubbard model even quantitatively, as shown in Fig.1.24(b), indicating the agreement with theory.
**Figure 1.23:** (Left) ARPES data for $SrCuO_2$. (a) Intensity distribution as a function of momentum at a constant energy. b). Raw ARPES data with $k_\perp = 0.7\text{Å}^{-1}$. c). Second derivatives are plotted to trace the peaks. (Right) EDCs and dispersions. (a). EDCs for $k_\parallel$ between $\Gamma$ to $0.6\pi$ at $k_\perp = 0.7\text{Å}^{-1}$. Each EDC is curve-fitted to find the peak positions. (b). Experimental (symbols) and theoretical (solid and dashed lines) dispersions. Dispersions from the band theory are also shown as two dotted lines. From Kim et al., 2006.

**Figure 1.24:** a). Schematic PES data of the doped 1D Hubbard model with band filling $\frac{1}{2} < n < \frac{2}{3}$. b). Dispersion results of the 1D Hubbard model calculated for $U = 1.96\text{eV}$, $t = 0.4\text{eV}$, and $n = 0.59$ in comparison to the ARPES dispersions for TTF-TCNQ. From Single et al., 2003.
1.3.5.2 Electronic structures of HTSC

The advancement of ARPES techniques unprecedentedly improve our understanding of the electronic structure of cuprates, by unveiling unexpected spectral features such as “high-energy kink” and “waterfall” and identifying the quasi-particle

“High-energy Kink” and “waterfall” : When people tried to explore the renormalization effects of many-body interaction at relatively high energies in cuprates, some anomalous high-energy dispersions were evidenced (Fig.1.25). In the nodal direction, the “high-energy kink” at $\sim 0.4eV$ is followed by a nearly vertical dispersion (“waterfall”) that ends up below 1eV and is very close to the unrenormalized bare band. This transfer of weight from low-energy to high-energy features indicates strongly correlation effects.

Evolution of quasi-particle peak : In cuprates, different phases can be realized by simply controlling the charge carriers doped into the $CuO_2$. It is widely believed that the keypoint of the HTSC puzzle in cuprates is to identify the “quasiparticle” that participate in the formation of Cooper pairs. By tunneling the doping, ARPES can provide evidence for the evolution of quasi-particle peak (see Fig.1.26): In the underdoped regime, no quasiparticle peak can be detected and the incoherent components are increased. This is consistent with conservation of the total spectral weight. In the overdoped case, a pronounced change in the ARPES spectral lineshape arises.
Figure 1.25: (Left) Intensity plot of ARPES data for \( \text{Sr}_2\text{CuO}_2\text{Cl}_2 \) along the \( \Gamma-(\pi,\pi) \) direction taken with 22.4eV photons as a function of momentum and binding energy (from [9]). The results are compared with the shifted dispersion from the LDA calculation (dashed line). (Right) Second derivatives of ARPES intensity maps along the node direction \((0,0) \rightarrow (\pi,\pi)\) of Pb2212 (a) and SrCuO\(_2\) (b). (c) and (d) show the MDCs and EDCs from data shown in panel (a) (from [10]). Here the dotted line and the dashed line highlight the proposed spinon and holon dispersion, respectively.

Figure 1.26: a),b). ARPES dispersion in YBCO, along the nodal cut \([\Gamma \rightarrow (\pi, \pi)]\) for \( p = 0.24 \) (overdoped) and \( p = 0.06 \) (underdoped). c). \( A(k=k_F, \omega) \) as a function of doping for the bonding Cu-O band, showing the progressive suppression of the quasiparticle peak.
Chapter 2

Numerical Methods

Although models for strongly correlated systems can vastly simplify the complications in the real materials and capture the essence of the physics we care about, seeking their analytical solutions is usually quite challenging. Various assumptions and approximations can be adopted, but their validity might be questionable and can be out of control. Numerical methods as a separate approach can be regarded as a complementary access to tackle various models. Various numerical methods [36–68] have been applied to strongly correlated systems. The majority of these methods can be grouped into three categories: (i) exact, (ii) variational, (iii) stochastic.

In the group (i) we include exact diagonalization techniques. The basic idea essentially consists of exactly solving the Schrödinger equation by brute force. Since it can obtain all energy levels of the finite system under study, all properties can be calculated in principle. However, the Hilbert space, or in other words, the size of the basis needed to represent the Hamiltonian, grows exponentially with the size of the systems, limiting their applicability to the study of relatively small systems. By adopting some symmetries and efficient numerical methods, such as Lanczos algorithm, to generalize the size of system, the extension of the capability is still limited. As a result, exact diagonalization fails to describe the properties of system in the thermodynamic limit.
Variational methods rely on an ansatz: a proposed wave-function derived from some physical grounds. If the wave-function describes the actual ground state of the system, even in an approximate way, it may contribute enormously to our knowledge of the system. For one dimensional systems, the Bethe ansatz is actually exact when applicable. The BCS theory of superconductivity also relies on a variational ansatz, that is origined from a mean-field treatment.

Quantum Monte Carlo techniques are based on the stochastic sampling of the Hilbert space using random walks. These methods are extremely powerful, being able to study very large systems at finite temperature. However, they suffer from the so-called “minus-sign problem”, which arises from the fermion statistics. This limits their applicability to “unfrustrated models”.

2.1 The Density Matrix Renormalization Group (DMRG)

The Density Matrix Renormalization Group (DMRG) method [69–71] is a very powerful numerical method able to treat very large systems with hundreds of degrees of freedom (e.g. spins, electrons), and to provide extremely accurate results for ground-state energies and gaps in low dimensional systems. Since its very early days the DMRG has shown spectacular success and, together with Quantum Monte Carlo, has dominated most of the numerical research in the field.

In a certain way, DMRG can be thought of as an algorithm to compress the wave-function, same as classical compression algorithm work in digital imaging: The ground state of one-dimensional system can be parameterized by a number of coefficients that is much smaller than the dimension of the Hilbert space. In other words, only a relevant subset of states of the full Hilbert space needs to be considered to simulate ground state properties of the system. In a typical renormalization
procedure of Hamiltonian, microscopic Hamiltonian is initially represented in a particular basis and degrees of freedom are iteratively added, typically by increasing the size of the finite system. To control the complexity of the problem, less important parts are integrated out by modifying the original Hamiltonian and some set of couplings newly generated by the elimination of degrees of freedom will be truncated based on some physical motivations. When some criterion is fulfilled, we can obtain a simplified effective Hamiltonian that is supposed to capture the essential physics of the system under study. This is the essence of the so-called “real space renormalization group” introduced by Wilson. The difficulty and glory of the method revolves around how reliably the truncation is performed. For instance, the original Numerical Renormalization Group (NRG) is based on the assumption that the ground state of the entire system can essentially be composed of energetically low-lying states living on smaller subsystems (the forming blocks). So it eliminates high-energy eigen-states in each iteration and achieved great success when applied for quantum impurity problem. However, it fails in the description of strongly interacting systems, such as Hubbard model. To solve the breakdown of NRG, a convenient strategy is to embed the finite system in some environment that mimics the thermodynamic limit of the system. This triggers the birth of the DMRG. In the following, we will briefly review the basic structure of the infinite- and finite-system DMRG for one-dimensional lattice systems.

2.1.1 Infinite-system DMRG

In the infinite system algorithm, we keep enlarging the system until the ground state properties we are interested in (e.g. the ground state energy per site) have converged. Each iteration mainly consists in two steps: building the superbblock and renormalization procedure.
Building the superblock: To build the superblock, we need to first build the block \( B(L,m_L) \) that contains all the information about the block: the block Hamiltonian \( \hat{H}_B \), its basis and other relevant operators. The arguments of \( B \) refer to the number of sites it contains and to the number of states used to describe it, respectively. Then we need to build the left enlarged block by adding a new site to the right of the previous block and create the associated Hamiltonian \( \hat{H}_{LE} \) that involves the individual Hamiltonians for the block and the added site, respectively, plus their interaction term

\[
\hat{H}_{LE} = \hat{H}_B + \hat{H}_S + \hat{H}_{BS}
\]

To embed the system in the environment, the enlarged block is then coupled to a similarly constructed right enlarged block and the superblock is obtained

\[
\hat{H}_{\text{superB}} = \hat{H}_{LE} + \hat{H}_{RE} + \hat{H}_{SS'}
\]

Here the left enlarged block is treated as the system under study and right one plays the role of environment.

Renormalization procedure: To renormalize the system, the superblock Hamiltonian \( \hat{H}_{\text{superB}} \) should be diagonalized to find the ground state, which is denoted by \( \Psi_G = \Psi_{aab\beta} \). Here Latin indexes indicate blocks, while Greeks indexes refer to newly added sites. Obviously, the state of the system under study can be represented by the reduced density matrix \( \rho_L \)

\[
\rho_L = Tr_R [\Psi_G] \langle \Psi_G | = \sum_{b\beta} \Psi^*_{aab\beta} \Psi_{a'a'b'\beta} |a'a\rangle |a\rangle = \sum_{\lambda=1}^{\chi} a_{\lambda} |\lambda\rangle \langle \lambda|
\]

where the reduced density matrix is diagonalized further using singular value diagonalization (SVD), \( |\lambda\rangle \) denotes the Schmidt basis and \( \chi \) represents the Schmidt
rank that is bounded by the smaller dimension of the Hilbert space of the two super blocks. These eigenvalues $\lambda$ are related to the entanglement and weight the contribution of the associated basis to the ground state. Obviously truncation of this basis leads to the information loss of the representation. So we have to make a good balance between complexity and accuracy: these basis are arranged in a descending order according to their weights, only a fixed number $m$ of states with maximum weights are kept and all the rest are ignored. This corresponds to a truncation of the Hilbert space of the enlarged block. It provides a controllable way to find an efficient representation of the ground state. In other words, the truncation is based on the entanglement not the energy. Accordingly, all relevant operators including the block Hamiltonian should be renormalized by rotating the basis. The infinite-DMRG algorithm can be summarized in Fig.(2.1)

![Figure 2.1: Schematic procedure for the infinite DMRG algorithm. The algorithm starts from the system block $B(L,m_L)$, which couples with one site to form the enlarged block $B(L,m_L)$. If the reflection symmetry is present, the environment can be represented a right block that is a reflection of the left enlarged block. To embed the system into the environment, we can create the superblock $B(L,m_L) \cdot B(L,m_L)$ by coupling these two enlarged blocks together. After a renormalization procedure, we can obtain the new block for the next iteration.](image)

As an example, we can apply the infinite DMRG to Heisenberg chain (as shown in Fig.(2.2)) and plot the error of energy per bond as a function of iterations for different states to keep. The output shows that the accuracy can be improved by the number of states kept in the simulation.
2.1.2 Finite-system DMRG

The above infinite-system DMRG does not converge to the thermodynamic limit, since the configuration of ground state at infinite size will not be the low energy configuration at infinite size, especially the Hamiltonian changes at each step. This has to be improved by iteration self-consistently. To obtain the thermodynamic limit accurately with DMRG, the proper approach is studying finite systems and performing a finite-size analysis. The finite-system DMRG is the finite-size algorithm on systems of fixed length, and mainly consists in two steps: Reaching the desired size and a sweeping procedure.

Reaching the desired size : The infinite-system DMRG algorithm is adopted to grow the system until the superblock reaches the desired length $L_0$. So the final configuration of the system becomes $B(\frac{L_0}{2}-1,m)\cdots B(\frac{L_0}{2}-1,m)$.

Sweeping procedure : To improve the accuracy, we need to perform sweeps from left-to-right and right-to-left. During a left-to-right sweep, the left block is enlarged with one site and the right one is reduced correspondingly in order to keep the length $L_0$ fixed. So after one finite-system step the system configuration
becomes $B(\frac{L_0}{2}, m) \cdot B(\frac{L_0}{2} - 2, m)$. This can be done by renormalizing the left block and using the right block from the infinite-system step, or from the previous right-to-left sweep. This procedure continues until the length of the left enlarged block reaches $L_0 - 4$, so the final configuration of the system after the first sweep becomes $B(L_0 - 3, m) \cdot B(1, D)$ and the approximate ground state wavefunction can be improved. To improve the accuracy further, we can switch the role of the left and right enlarged blocks, and sweep from right to left. Usually sufficient convergence can be achieved after several sweeps. The finite-DMRG algorithm can be summarized in Fig.(2.3)

![Diagram of the DMRG algorithm](image)

**Figure 2.3:** Schematic illustration of a complete finite-system DMRG sweep.

As an example, we can apply the finite DMRG to finite Heisenberg chain with $L=24$, and calculate its ground state energy for different number of states kept and number of sweeps. Given the number of states kept, the errors of energies in Fig.2.4 converges with the number of sweeps as expected. Here the exact value is given by the Bethe Ansatz.
The time-dependent DMRG [71–73] is a new variant of the Density Matrix Renormalization Group method to solve the time-dependent Schrödinger equation, enabling one to simulate real-time dynamics of strongly correlated systems with unprecedented accuracy. It can be used to calculate spectral functions, and to study systems far from equilibrium by solving the time-dependent Schrödinger equation.

The problem consists of simply solving the following time-dependent Schrödinger equation:

\[
    i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle
\]

which has a formal solution

\[
    |\Psi(t)\rangle = \hat{U}(t)|\Psi(t = 0)\rangle
\]

Here the operator \( \hat{U}(t) = e^{-i\hat{H}t/\hbar} \) is the time-evolution operator. If we know the eigenvalues \( E_n \) and eigenstates \( |n\rangle \) of the Hamiltonian \( \hat{H} \), the initial state can be
expressed as:

$$|\Psi(t = 0)\rangle = \sum_n c_n |n\rangle$$

and the solution to our problem is simply given by:

$$|\Psi(t)\rangle = \sum_c c_n e^{-i \frac{E_n t}{\hbar}} |n\rangle$$

In small systems, where full diagonalization of the Hamiltonian is viable, this solves our problem. However, in DMRG one works in a basis with the form of matrix product states, and in this basis the coefficients will be wildly oscillating functions of time with different frequencies. On top of that, one is working in a truncated basis that does not account for the full Hilbert space. Our wave-function may evolve in time and may “explore” or “drift” toward regions of the Hilbert space that we have not properly accounted for. So the challenge is to adapt our basis as time evolves, such that at every time-step, our wave-function is optimized to represent the actual exact solution of the time-dependent Schrödinger equation, in the same spirit as the original DMRG. This is the main idea behind the “adaptive” tDMRG scheme, in which one variationally optimizes the wave-function as it evolves in time.

### 2.2.1 Spectral properties using the time-dependent DMRG

The knowledge of the excitation spectrum of a system allows one to make direct comparison with experiments, such as photoemission, or neutron scattering, for instance. The numerical evaluation of dynamical correlation functions is a very difficult task, and most methods usually are only capable of calculating the ground-state, and maybe some low energy excitations. A number of techniques have been used in the past, but they all have very important limitations: exact diagonalization is limited to small clusters, quantum Monte Carlo suffers from the sign problem,
and requires uncontrolled analytic continuations and the use of the max entropy approximation, and dynamical DMRG is computationally very expensive.

For a decade or more, these limitations have in part prevented much progress in this area. However, our time-dependent DMRG method has the potential to tackle many open problems, due to its versatility and for being computationally less intensive. From accurate calculations of time-dependent correlation functions, one can extract the single particle Green’s functions, and the entire spectrum of excitations in a single run, and with modest computational resources. This technique has been used to a number of problems, such as the partially spin-polarized one-dimensional Hubbard chain and spin-incoherent Luttinger liquids.

Imagine that we want to calculate a time-dependent correlation function that looks like

\[ G(t) = \langle \psi | \hat{B}(t) \hat{A}(0) | \psi \rangle \]

where \( | \psi \rangle \) is the ground state of the Hamiltonian \( \hat{H} \), and \( \hat{B}(t) = \exp(i \frac{Ht}{\hbar}) \hat{B}(0) \exp(-i \frac{Ht}{\hbar}) \).

If we are interested in obtaining the full momentum-resolved spectrum, we would want to calculate a correlator

\[ G(x' - x, t' - t) = i \langle \hat{O}(x', t') \hat{O}(x, t) \rangle \]

where \( \hat{O} \) is an operator of interest. In practice we apply the operator \( \hat{A} = \hat{O}(x = \frac{L}{2}) \) at the center site at time \( t = 0 \) to obtain \( | \phi \rangle \), and apply \( \hat{B} = \hat{O}(t') \) on all the sites \( x' \) at every time step. This will yield the correlations in real space and time. Fourier transforming of these functions to momentum and frequency, will then yield the corresponding spectral weights as functions of momentum and frequency:

\[ A(k, \omega) = \sum_n |\langle \psi_n | \hat{O}_k | \psi_0 \rangle|^2 \delta(\omega - E_n + E_0) \]
where $E_0$ is the ground state energy, and the sum runs over all the eigenstates of the system, with energy $E_n$.

If we are interested in obtaining the ARPES spectrum, we would want to calculate the one-particle Green’s function

$$G(x' - x, t' - t) = i\langle \psi_0| T[\hat{c}^\dagger(x', t')\hat{c}(x, t)]|\psi_0 \rangle$$

where $|\psi_0 \rangle$ is the ground state of the Hamiltonian $\hat{H}$, and $\hat{c}(x, t) = \exp(i\frac{Ht}{\hbar})\hat{c}(x, 0)\exp(-i\frac{Ht}{\hbar})$.

As an example, we can apply the time-dependent DMRG to calculate the spectral function of the Hubbard chain at half-filling (shown in Fig. 2.5). Obviously, it has a rather high resolution so that we can clearly identify the high-frequency features including the shadow band (E), in addition to the spinon (A) and holon bands (B) including its mirror component (D), which displays the spin-charge separation as predicted by Luttinger liquid theory. Note that all holon bands and shadow band disperse with period $\pi$, indicating the presence of local AF correlations [49].

![Figure 2.5: a). Spectral function A(k,ω) for Hubbard chain at half-filling by t-DMRG. Its Hubbard subbands separated by U are related to each other by the particle-hole symmetry.](image)
2.3 Quantum Correlations: Entanglement and Quantumness

Since the birth of quantum mechanics, people posed a question: “can we explain quantum mechanics in classical terms?” Later, quantum correlations are proposed to represent correlations in quantum systems, that cannot be explained by classical physics. According to research on entangled particles (such as EPR paradox, Bell’s inequality) and quantum measurement, it was realized that “spooky action at a distance” – referred-to as entanglement – exists and is responsible for quantum correlations. The rise of quantum information theory in the 1990’s realizes that this intrinsic feature of quantum physics opens the door to novel communicational and computational possibilities and much effort has been devoted to understanding its classification, measurement and quantification. At the same time, it was found that entanglement did not account for all quantum correlations: Quantum correlations beyond entanglement, such as “discord”, indeed exist. During the last two decades, both entanglement and discord have been applied to condensed matter physics: their analysis in quantum system –especially in strongly correlated systems– can essentially characterize quantum matter and their quantum phase transitions. Currently, they can be understood in two separate paradigms: separability vs. quantumness. In the following, we will explain these two concepts in the context of (quantum) information theory and take the bipartite system (a joint quantum system composed of subsystem A and B) as example.

2.3.1 Separability and Entanglement

The most remarkable feature of quantum mechanics that distinguishes it from classical physics is that for any composite system, there exists pure states of the system in which the parts of the system do not have pure state of their own. To be concrete, we just focus on a bipartite state: A joint system composed of subsystems A and B
is separable if its state $\rho$ can be represented as a mixture of product states

$$\rho^{AB} = \sum_i p_i |\phi_i^A \rangle \langle \phi_i^A| \otimes |\phi_i^B \rangle \langle \phi_i^B|$$

(2.1)

with \{p_i\} a probability distribution, $|\phi_i^A \rangle \langle \phi_i^A|$ and $|\phi_j^B \rangle \langle \phi_j^B|$ families of density matrices for subsystem $A$ and $B$, respectively. Otherwise, $\rho$ is entangled.

**Entanglement Measure for pure states—entanglelement entropy** : Entanglement in pure states can be measured through the entanglement entropy by means of the Schmidt decomposition. For instance, let us consider an arbitrary 2-qubit state: $|\psi_{AB} \rangle$. In the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, we can choose an orthonormal basis \{|e_i \rangle \otimes |e_j \rangle\} for the space in terms of which the state can be represented as

$$|\psi_{AB} \rangle = \sum_{i,j=1}^{d_A,d_B} A_{ij} |e_i \rangle \otimes |e_j \rangle$$

In general, $d_A \neq d_B$, but we can diagonalize it via SVD and obtain

$$|\psi_{AB} \rangle = \sum_{\alpha=1}^{r} a_{\alpha} |\tilde{e}_\alpha \rangle \otimes |\tilde{e}_\alpha \rangle$$

where $|\tilde{e}_\alpha \rangle = U_{\alpha i} |e_i \rangle$, $|\tilde{e}_\alpha \rangle = V_{\alpha j} |e_j \rangle$ and $a_{\alpha} = U_{\alpha i} A_{ij} V_{j\alpha}$. The reduced density matrices for its subsystem $A$ can be obtained by tracing over the subsystem $B$

$$\rho_A = Tr_B[\rho_{AB}] = \sum_{\gamma=1}^{r} (1_D \otimes |\tilde{e}_\gamma \rangle)(\sum_{\alpha,\beta=1}^{r} a_{\alpha} a_{\beta} |\tilde{e}_\alpha \rangle \otimes |\tilde{e}_\alpha \rangle \langle \tilde{e}_\alpha| \otimes \langle \tilde{e}_\beta| \otimes \langle \tilde{e}_\gamma|)(1_D \otimes |\tilde{e}_\gamma \rangle) = \sum_{\alpha=1}^{r} a_{\alpha}^2 |\tilde{e}_\alpha \rangle \langle \tilde{e}_\alpha|$$

, which leads to the von Neumann entropy

$$E(\rho^A) = - \sum_{\alpha=1}^{\chi} a_{\alpha}^2 \log_2 a_{\alpha}^2$$

Here $r$ represents the Schmidt rank. When $r = 1$, i.e. it has only one non-vanishing coefficient $a_i$, then the pure state $|\psi_{AB} \rangle$ is a separable state. In this situation, the
associated state of the subsystem is a product state, as expected. Therefore, the Schmidt decomposition provides a necessary and sufficient criterion for separability of pure states.

**Entanglement Measure for mixed states—entanglement of formation**: For mixed states, no such an elegant decomposition exists. How to quantify the entanglement of a mixed state of a bipartite system is a complicated problem and has attracted a lot of attention in the quantum information community. Different measurements have been proposed to quantify the entanglement in bipartite states, including entanglement of formation, negativity, relative entropy of entanglement and so on. Here we just focus on *entanglement of formation*, which is one of the most popular and frequently used measures. Physically, it is defined as the minimal number of pure states needed to create a single copy of the mixed state that represents $\rho$. Given a mixed state $\rho$ of a bipartite system, consider its all possible pure states decomposition. That is, we consider states $\{|\psi_i\rangle\}$ and associated probabilities $p_i$ such that

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

The entanglement of formation of $\rho$, $E(\rho)$, is defined as the minimal, over all such ensembles, of the average entanglement of the pure states making up the ensemble

$$E(\rho) = \min_{p_i,|\psi_i\rangle} \sum_i p_i S(|\psi_i\rangle)$$

where $S(|\psi_i\rangle)$ is the von Neumann entropy, and the minimization is over all pure state decompositions. For pure state, only one $p_i$ is nonvanishing, meaning it reduces to the conventionally von Neumann entropy. In general, the separability problem is NP-hard, but for the mixed state of the two-spin system, the separability is determined by the Peres Horodecki (PPT) criterion, which tells us that the necessary and sufficient condition is that the partial transpose of $\rho^{AB}$ with respect to spin “B”
has non-negative eigenvalues. In a seminar paper [74], Hill and Wooters found a closed formula for the entanglement of formation for two spins

\[ E(\rho) = h\left(1 + \frac{\sqrt{1 - C(\rho)^2}}{2}\right) \]

with

\[ h(x) = -x \log_2 x - (1 - x) \log_2 (1 - x) \]

The quantity \( C(\rho) \) is called the “concurrence” and has the property that it is an entanglement monotone and is zero for a separable state. For a mixed state of two spins/qubits, it takes the form:

\[ C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4) \]

where the \( \lambda_i \)'s are the square roots of the eigenvalues of the matrix \( \tilde{\rho} \rho^\dagger \) in decreasing order, with

\[ \tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^\dagger(\sigma_y \otimes \sigma_y) \]

is the complex conjugate of \( \rho \) in the standard basis \( |\sigma, \sigma'\rangle \), and \( \tilde{\rho} \) represents the spin-flipped state.

### 2.3.2 Quantumness and Quantum Discord

In quantum systems, a measurement on a single subsystem can alter the global correlations. This feature is also pure quantum with no classical counterpart: Correlations in classical system remain unaltered by measurement on a subsystem. Based on the classicality/quantumness of correlations, a different paradigm arises [75]. A mixed state shared by two parties, \( A \) and \( B \), is a classically correlated if the density
matrix can be written as

\[ p_{cc} = \sum_{i,j} p_{ij} |i^A\rangle \langle i^A| \otimes |j^B\rangle \langle j^B| \]

where \{\langle i^A\rangle\} and \{\langle j^B\rangle\} are orthgonormal states on A and B, and the probabilities \( p_{ij} \) are nonnegative, and \( \sum_{i,j} p_{ij} = 1 \). Otherwise, the state is called quantum correlated. A classically correlated state can be called classical-classical state and is also separable, but a separable state (refer to eq.(2.1)) is not necessarily classically correlated, since the states \{\langle i^A\rangle\} and \{\langle j^B\rangle\} do not have to be orthogonal. Moreover, a pure state is quantum correlated if and only if it is entangled, i.e. for pure states both paradigms are equivalent. To quantify the quantumness of a quantum system, we can introduce the measure of quantum discord. But before that, we quickly review some relevant concepts in classical information theory.

**Mutual information in classical theory**: In classical information theory, correlation between two random variables \( X \) and \( Y \) can be measured by the mutual information \( I(X:Y) \), which can be expressed in two ways, namely

\[
I(X : Y) = H(X) + H(Y) - H(X,Y) \\
I'(X : Y) = H(X) - H(X|Y)
\]

Here \( H(X) \) represents the Shannon entropy describing the ignorance about a random variable \( X \), given by

\[
H(X) = - \sum_x (p_{X=x}) \log(p_{X=x})
\]

where \( p \) is the classical distribution followed by \( X \), and \( H(X,Y) \) is the joint entropy of both variables \( X \) and \( Y \). \( H(X|Y) \), the conditional entropy of \( X \) given \( Y \), is
defined as

\[ H(X|Y) = \sum_y p_y H(X|Y = y) \]

with \( H(X|Y = y) = -\sum_x p_{x|y} \log p_{x|y} \). \( I \) and \( I' \) are equivalent for classical random variables due to Bayes’ rule \( p_{x|y} = \frac{p_{xy}}{p_y} \), which can be used to show that \( H(X|Y) = H(X,Y) - H(Y) \).

**Mutual information in quantum theory and quantum discord**: For a quantum state with the density operator \( \rho^{AB} \), the mutual information \( I(\rho^{AB}) \) between \( A \) and \( B \) is given by

\[ I(\rho^{AB}) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}) \]

with the von Neumann entropy \( S \), and the reduced density operators \( \rho^A = Tr_B[\rho^{AB}] \) and \( \rho^B = Tr_A[\rho^{AB}] \). It is the generalization of the classical mutual information \( I(X:Y) \) to the quantum theory. On the other hand, the generalization of \( I'(X:Y) \) is a little tricky: The conditional entropy of \( A \) conditioned on a measurement on \( B \) is

\[ S(A|\{\pi_i^B\}) = \sum_i p_i S(\rho_i^A) \]

where \( \{\pi_i^B\} \) are orthogonal projectors with rank one on the subsystem \( B \), \( p_i \) is the probability for obtaining the outcome \( i \) given by \( p_i = Tr[\pi_i^B \rho^{AB}] \), \( \rho_i^A \) represents the post-measurement state of the subsystem \( A \) given by \( \rho_i^A = \frac{Tr_B[\pi_i^B \rho^{AB}]}{p_i} \). So the quantity \( I' \) can be extended to quantum states as follows

\[ I'(\rho^{AB}) = S(\rho^A) - S(A|\{\pi_i^B\}) \]

whose values generally depends on the choice of \( \pi_i^B \). Physically, it represents the amount of information extracted about the subsystem \( A \) by measuring the subsystem
B. *Quantum discord* can be defined as the difference of these two inequivalent expressions for the mutual information, minimized over all possible $\pi^B_i$:

$$D(\rho^{AB}) = \min_{\pi^B_i} [I(\rho^{AB}) - I'(\rho^{AB})_{\{\pi^B_i\}}]$$

It vanishes if and only if the state is classical-quantum or quantum-classical, i.e. the state is quantum correlated. It has been found that quantum discord is more robust than the entanglement in the sense that almost all bipartite quantum states have a non-vanishing quantum discord that can remain nonzero under almost all quantum evolution.

### 2.3.3 Modern understanding of DMRG

For a long time, the use of DMRG has been rather empirical in the sense that there has not been a clear criterion to access the convergence of the method and to determine when the truncation should be done. The occurrence of the breakthrough was yielded by quantum information [76] that has provided a more rigorous framework to understand when and why the DMRG algorithm will succeed.

According to quantum information theory, DMRG can be thought of a variational approach that is based on the Matrix Product State (MPS) ansatz provides an extraordinary good approximation to the ground state of most (finite) 1D gapped Hamiltonian with finite-range interactions at zero temperature. Such ground states fulfill generally a so-called ‘area law’, which indicates that for a given system, the entanglement between a part of the system and the rest of the system depends on the boundary of the block rather than on its volume. As mentioned above, truncation errors due to disentangling the left and right blocks in DMRG characterize the loss of quantum information. What DMRG really does is to minimize the loss of information: The more Schmidt weights are ignored, the more quantum information is lost. In general, the number of DMRG states that we need to keep to represent a
state is related to the entanglement entropy between the two blocks \[77\] as

\[ m \approx \exp(S) \]

where \( S \) denotes the entanglement entropy between the two blocks.

According to the study of the entanglement properties of quantum systems \[71\], entanglement entropy of certain classes of system has been understood:

- Gapped systems in 1D: \( S=\text{const} \rightarrow m=\text{const} \)
- Critical systems in 1D: \( S \sim \log L \rightarrow m \approx L^\alpha \)
- Gapped systems in 2D: \( S \sim L \rightarrow m \approx \exp(L) \)

Obviously, the entanglement entropy of a gapped 1D system remains constant being independent of the size of the system \( L \), meaning that the number of DMRG state \( m \) remains independent of \( L \) as well, as long as \( L \) is larger than the correlation length. If the system becomes critical, the entanglement entropy receives a logarithmic correction, so \( m \) grows polynomially with \( L \). For a gapped 2D system, the entanglement entropy \( S \) is proportional to \( L \), indicating that \( m \) grows exponentially with \( L \). Therefore, the validity of DMRG algorithm relies on the fact that these states are characterized by a number of parameters that scales only polynomially with the number of sites and not exponentially.
Chapter 3

Cluster Perturbation Theory (CPT) with DMRG as a solver

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3.1 Introduction

Since the discovery of high temperature superconductivity in lightly doped antiferromagnets such as doped cuprates, a lot of attention has been focused on the doped Mott insulators. As typical examples of strongly correlated systems, they defy conventional paradigms, since the rigid band picture behind the physics of semiconductors does not apply: in strongly interacting systems, the bands change with doping, giving rise to a complex phenomenology especially near the Mott transition. With the development of advanced experimental techniques, such as ARPES, various exotic electronic properties including hole pockets, Fermi arcs, kinks [9, 10, 20, 21] have been revealed. On the other hand, the spectral properties near the Mott transition in the Hubbard model have been studied extensively by a number of computational
techniques [36–68], such as exact diagonalization (ED), quantum Monte Carlo simulation (when the sign problem does not occur), density matrix renormalization group (DMRG) (in 1D) and results indicate the emergence of excitations in the Mott gap at finite doping. The “leaking” of spectral weight into the gap has been explained a while ago by the seminal work by Eskes et al [78] and reviewed in Ref.[79]

Previous numerical studies using cluster perturbation theory (CPT) [51] indicate the survival of one-dimensional aspects in the spectrum of the fully two-dimensional systems, and suggest that some of the features observed in the experiments, such as kink or waterfalls [20], could be attributed to spin-charge separation and traced back adiabatically to spinon and holon dispersion in one-dimensional chains. Even though spin-charge separation is intrinsically a manifestation of 1D physics, the possibility of its presence in two dimensions or quasi-two-dimensional (quasi-2D) systems has been extensively debated, particularly within the context of high-temperature superconductivity [80]. Some numerical studies in this direction, looking at two, three, and four-leg $t - J$ ladders, indicate the presence of spinon and holon excitations [81–85]. Whether spin-charge separation, or electron-phonon interactions are responsible for the unexpected spectral features such as kinks, and “waterfalls” in cuprates, has deserved greate debate and remains open to interpretation.

In this chapter, we want to apply tDMRG as a solver for CPT to study the two-dimensional one-band Hubbard model, at and away from half-filling. As mentioned above, the DMRG itself is hard to apply to 2D strongly correlated systems directly and the CPT fails to capture intermediate- and long-range dynamical correlations (see below). We expect that the combination of tDMRG and CPT can be a powerful tool to study the 2D Hubbard model. Furthermore, the one-band Hubbard model can effectively describe the $CuO_2$ plane of high-$T_c$ cuprate materials after the oxygen degrees of freedom are eliminated via the Zhang-Rice construction [34], so the spectral function of one-band Hubbard model can provide us with information about the electronic properties of Cuprates.
3.2 Methods

3.2.1 Cluster Perturbation Theory (CPT)

Cluster Perturbation Theory (CPT) is a technique that applies to problems with local interactions, such as the Hubbard model [49, 51, 86], or models where the local interaction is predominant. It provides an approximation to the single-particle Green’s function of the problem in the thermodynamic limit by coupling clusters of small size in a variant of strong coupling perturbation theory. The main idea consists in dividing the lattice into identical small clusters which can be solved exactly using some numerical techniques, such as exact diagonalization (ED), and coupling them together to reconstruct the original system.

For instance, given a lattice \( \gamma \), we divide it into a superlattice \( \Gamma \) of identical clusters of \( L \) sites each as shown below in Fig.(3.1)

![Figure 3.1](image)

This is equivalent to the decomposition of the Hamiltonian

\[
H = H_0 + V = \sum_{m \in \Gamma} H^{(c)}_m + \sum_{m,n \in \Gamma} H^{(i)}(m,n)
\]

where \( H_0 \) and \( V \) represent the kinetic and potential terms respectively, \( H^{(c)} \) only contains terms belonging to a single cluster, \( H^{(i)}(m,n) \) consists of the incluster...
hopping terms connecting the $m$th and $n$th clusters given by

$$H^{(i)}(m, n) = \sum_{a,b} t_{ab}^{mn} c_{m,a}^\dagger c_{n,b}$$

Here the hopping matrix $t_{ab}^{mn}$ is nonzero only for hopping processes across the boundaries of the cluster. The indices $m$ and $n$ denote the individual clusters, the indices $a$ and $b$ denote sites within a cluster. This decomposition explicitly breaks the translational invariance of the original lattice model, so we need to restore the translation invariance by periodization in the end.

The single-particle Green’s function for the thermodynamic limit is constructed by solving a simple Dyson-like equation:

$$G^{-1} = G'^{-1} - T$$

where the bold symbols represent matrices: $G$ is the Green’s function of the system we seek, $G'$ is the Green’s function in the cluster, and $T$ is a hopping matrix connecting the clusters. In the following, we will assume that the symbol $G$ refers to retarded Green’s functions, from which we can obtain the spectral function of the system which can be compared to ARPES data.

**Advantages of CPT**: The CPT becomes exact in both the non-interacting and strong-coupling limits, and provides an approximate interpolation between them. It has the advantage of allowing for a continuum of wavevectors while at the same time capturing short-range dynamical correlations. More precisely, short-range correlations within the cluster are treated exactly, while long-distance effect is treated at the RPA-like level. The accuracy of the approximation is controlled by increasing the cluster sizes.

**Disadvantages of CPT and its generalization**: CPT fails to describe long-range order, since it relies on the solution of small clusters, with typically 12-16
sites. This shortcomings can be overcome by using some extensions such as the variational cluster approximation (VCA). The VCA [53, 56] extends the previous ideas by incorporating additional ingredients, such as external fields or bath clusters and embeds the CPT into a formal framework, the so-called Self-energy-functional theory, which itself allows to derive non-perturbative and thermodynamically consistent approximations for lattice models of strongly correlated electrons from a general dynamical variational principle and provides a framework to unify several cluster methods based on their mathematical structure [87]. It has been exploited to determine the phase competition and the optimal symmetry-breaking fields [88–93].

3.2.2 CPT+tDMRG

We use the time-dependent DMRG [72, 73, 94, 95] as a solver for CPT and study the spectral function of the 2D Hubbard model with unprecedented resolution at and away from half-filling. The tDMRG can solve infinite (very large) one-dimensional system, so this combination allows us to couple clusters that already infinite (very large) in one spatial dimension, representing a great advance over traditional calculations with small clusters. In the following, our cluster consists of a $2 \times L$ ladder, and the model is given by the usual Hubbard Hamiltonian

$$H = -t \sum_{i,\sigma,\lambda} (c_{i,\sigma\lambda}^\dagger c_{i+1,\sigma\lambda} + H.c.) - t \sum_{i\sigma} (c_{i2\sigma}^\dagger c_{i1\sigma} + H.c) + U \sum_{i,\lambda} n_{i\lambda\uparrow} n_{i\lambda\downarrow}$$

where the operator $c_{i\sigma\lambda}^\dagger$ creates an electron on rung $i$ and leg $\lambda = 1, 2$ with spin $\sigma$, $n_{i\sigma\lambda}$ is the electron number operator, and $t$ and $U$ parameterize the hopping and Coulomb repulsion, respectively. To work with CPT, we assume periodic boundary conditions in the leg direction and open boundary conditions in the rung direction.

Since the cluster possesses translational invariance along the leg direction, we can readily Fourier transform the Green’s function in the cluster and obtain its hybrid
representation

\[ G''_{\lambda\lambda'}(k_x) = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ik_x n} G''_{\lambda\lambda'}(n) \]

where the leg index \( \lambda \) still represents a real space coordinate. We have omitted the spin index, since the problem is invariant under a spin inversion. As a result, for each value of \( k_x \), \( G \) is a \( 2 \times 2 \) matrix, which is exactly equivalent to solving the CPT equations for a two-site cluster, according to Eq.(3.1):

\[ G^{-1}_{\lambda\lambda'}(k_x, Q, \omega) = G'^{-1}_{\lambda\lambda'}(k_x, \omega) - T_{\lambda\lambda'}(Q) \]

with

\[ T_{\lambda\lambda'}(Q) = -t[e^{iQ}\delta_{\lambda,2}\delta_{\lambda',1} + e^{-iQ}\delta_{\lambda,1}\delta_{\lambda',2}] \]

and \( Q = 2k_y \) introducing the dependence on \( k_y \). Note that \( Q \) corresponds to the wavevector in the superlattice \( \Gamma \). By restoring the quasi-translational invariance, we obtain the CPT Green’s function as

\[ G^{CPT}_{\lambda\lambda'}(k_x, k_y, \omega) = \frac{1}{2} \sum_{\lambda', \lambda' = 1}^{2} e^{-ik_y(\lambda - \lambda')} G_{\lambda,\lambda'}(k_x, 2k_y, \omega) \]

. By reflection symmetry, we obtain \( G_{11} = G_{22}, G_{12} = G_{21} \), which reduces the number of required simulations.

**Some technique details** : To obtain the cluster Green’s function \( G' \), we can adopt the tDMRG method, which can yield the single-particle correlation function in real space and time, and the Green’s functions can be obtained by Fourier transforming the results to momentum and frequency. The most subtle aspect of this calculation concerns the use of open boundary conditions along the \( x \) direction. As discussed in Refs[72, 73, 96], the finite size effects introduced by the boundaries can be controlled in two ways: by convolving the Fourier transform to momentum.
space with a smooth window that vanishes at the boundaries, and by limiting the simulation time to prevent reflections at the two ends of the ladder. In addition, to avoid artifacts such as “ringing” in the Fourier transform to frequency, we also convolve the results with a Hann window along the time direction. Effectively, this might introduce an artificial broadening in the spectral function that is inversely proportional to the width of the time window. Long simulation time would reduce the broadening in frequency, with the price of introducing ringing. These features are amplified when the matrix is inverted and plugged into the CPT equation, introducing instabilities that result in negative values of the spectral function. Therefore, our simulation time (and Hann window width) is relatively short $t_{\text{max}} \sim 15$ in units of the inverse hopping and makes the use of linear prediction methods to extrapolate in time [97] completely unnecessary.

### 3.3 Results and discussion

#### 3.3.1 Spectral function of Hubbard ladder at half-filling

Now we simulate a $2 \times 80$ Hubbard ladder with 600 DMRG states, and use a time window of width $\Delta t = 15$, a time step $\delta t = 0.02$, and a third order Suzuki-Trotter decomposition of the evolution operator. In Fig.(3.2), we show results for the spectral function of the ladder, at half-filling and for $U/t = 8$, as a function of $k_x$, and for the symmetric and antisymmetric sectors, represented by $k_y = 0, \pi$, respectively:

$$G'(k_x, k_y = 0, \pi, \omega) = G'_{11}(k_x, \omega) \pm G'_{12}(k_x, \omega)$$

where the $\pm$ signs correspond to the two values of $k_y$. Since the cluster is gapped in both the charge and spin sectors, the truncation errors are very small, of the order of $10^{-7}$.  

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Even though ladders are quasi-one-dimensional systems with spin-charge separation and Luther-Emery behavior [98, 99], the sharp features observed in chains (shown in Fig.2.5), such as shadow and spinon bands, are washed out and becomes less discernible, with most of the spectral weight concentrated in the holon bands. The spinon band in the lower Hubbard band (LHB) for $k_y = 0$ shows a tendency to merge with the holon band and forms a single quasiparticle dispersion, as we would expect from a Fermi liquid. The dispersion presents a waterfall that resembles a discontinuity in the dispersion at $k_x = \frac{\pi}{2}$, and could be attributed to the hybridization between the charge and spinon modes, induced by the hopping along the rung. This should be related to the formation of rung-singlet pairs, since for large $U$ the rung hopping can yield a Heisenberg interaction between spins of the two leg, which tends to create rung singlet. The upper Hubbard band (UHB) displays a sharp spinonlike dispersion centered at $k_x = \pi$ with very small bandwidth. These features are reversed for $k_y = \pi$: Due to particle-hole symmetry, the bands are reflected about the Fermi energy and shifted in $k_x$ by $\pi$. 

**Figure 3.2:** Spectral function of a Hubbard ladder with $L = 80$ and $\frac{U}{t} = 8$, at half-filling, obtained with tDMRG. Panels (a) and (b) show the symmetric and antisymmetric sectors, respectively, which are related by particle-hole symmetry.
3.3.2 Spectral function of 2d Hubbard model at half-filling

By plugging $G'$ into the CPT equations, we can reconstruct the spectral function of the 2D Hubbard model at half-filling with $\frac{U}{t} = 8$. If we plot the spectral function along the $\Gamma \to X \to M$ path in the Brillouin zone, we obtain very limited resolution along the $X \to M$ line since the cluster in the transverse direction is rather small. However, in a rotational invariant lattice, this spectral should be identical to the results for the $k_y = \pi$ boundary of the Brillouin zone, which can be obtained with very high resolution. For this reason, we have plotted the CPT spectrum for the $k_y = \pi$ along the $X \to M$ segment in Fig.3.3(a), with the price of introducing an artificial discontinuity at the $X$ point.

The spectral shows an uncanny resemblance to the ladder’s, albeit with a weak renormalization. As explained in [11], the CPT introduces a shift of spectral weight.
at high energies while keeping the spectral weight near the Fermi level almost unaffected, which make the holonlike bands sharper and the spinonlike bands weaker, yielding a dispersion that resembles that of quasiparticles. The spinon features remain as an incoherent background at low energies, while preserving the waterfall at \((\frac{\pi}{2}, \frac{\pi}{2})\).

Following \cite{100}, the quasiparticle dispersion can be fitted by a mean-field (Hartree-Fock) dispersion assuming a Neel antiferromagnetic (AFM) order \cite{100, 101}, given by the two bands

\[
E_{\pm}(k) = \pm \sqrt{[-2\tilde{t}(\cos k_x + \cos k_y)]^2 + \tilde{\Delta}^2}
\]

as shown by the dashed line in the figure, where we take the gap \(\tilde{\Delta}\) and \(\tilde{t}\) as free fitting parameters. This indicates that, despite its low dimensionality, the ladder cluster already introduces features in the spectrum that contain information about the onset of AFM order. Moreover, the spectral function displays a remarkable agreement with the quantum Monte Carlo (QMC) results from \cite{100, 102-104} but with much better resolution. In particular, we observe similar features such as the flat dispersion in the UHB and LHB centered at the \((\pi,0)\) point, and the weak spinonlike incoherent background at low energies. The high-energy “bands” observed in QMC can be associated to the shadow bands in the ladder dispersion, echoes of one-dimensional physics. Remarkably, these same features are also obtained using square clusters with CPT \cite{51} and VCPT \cite{88, 89}, after introducing an external staggered field to induce antiferromagnetic correlations in 2D clusters. Putting together the result from this and previous work, the evidence indicates that (i) these features are not artifacts of the quasi-one-dimensional ladder, and (ii) they survive in the presence of long-range order.
3.3.3 Spectral function of 2d Hubbard model away half-filling

Now we shift our attention toward the doped case. In Fig.(3.4), we show a similar calculation for

![Figure 3.4](image)

Figure 3.4: (a). CPT spectral function of the doped U = 8 2D Hubbard model obtained using a 2×40 ladder as a cluster, with n=72 electrons. (b). Same results focusing on the kink and the pseudogap region along the Γ → X line. (c). Pseudogap at the X point.

a 2 × 40 ladder with 72 electrons, corresponding to 10% doping, which also keeps us away from any charge-density wave instabilities. Here we use a smaller cluster and more states (m=1000), since the charge sector away from half-filling is gapless and introduces more entanglement in the problem, making the simulations computationally more expensive.

The spectrum looks very similar to the CPT results in small clusters [51] (see Fig.3.5(a)): the waterfall is no longer a discontinuity but a continuous feature resembling a “kink”, and there is clear transfer of spectral weight above the Fermi energy centered around the M point. This kink is identical to the one obtained
Figure 3.5: Doped spectral function obtained by other methods: a). Spectral function for $\delta = 0.07$ obtained using CPT (from [11]); b). (color) The DCA results of the spectral weight for $T = 0.14t$, $U = 8t$ and $n = 0.80$ using a 16 site cluster. A kink followed by a broad waterfall feature is noticed below $E_{\text{kin}} \approx t$. The thin line indicates the bare dispersion $E(k)$ (from [12]). c). The spectral function near the chemical potential in the 2D Hubbard model at $T = 0.088t$ and $U = 8t$ calculated with DCA/QMC for a 4-site cluster (from [13]).

with the DCA in [105]. In addition, our results show an additional “splitting” of the bands below and above the Fermi energy along the $k_y = 0$ line and centered at around the $X$ point. This splitting is accompanied by an additional kink at the Fermi surface, which appears at the onset of a branch of excitations that could be traced back to the upper branch of the spinon-antiholon continuum in the one-dimensional Hubbard model [11, 106]. Remarkably, these features also appear in the DCA calculations [13] which in principle should not have any “memory” of 1D physics and spin-charge separation. The splitting can be interpreted as a pseudogap, as we can clearly see in a cut along the frequency axes in Fig.3.4(c), in agreement with previous observations. This is different from what was observed in the CPT calculations on $4 \times 4$ clusters [51], that shows instead a flat dispersion, similar to the one observed in the undoped case.
3.4 Conclusion

In this chapter, we studied the spectral properties of the 2D Hubbard model using the tDMRG method as a cluster solver for CPT. Our clusters are “infinite” (very long) two-leg ladders, which already contain information about the thermodynamic limit along the leg direction. In addition, finite-size effect of charge fluctuations inside the clusters are largely reduced due to the large size of the ladders, so the results show a remarkable resolution of the bands in frequency and momentum and allow us to identify features such as waterfalls, kinks, and pseudogap, of significance in the physics of cuprate superconductors. These different aspects can be related to one-dimensional physics that survives, even in the presence of AFM correlations. Since these features also present in other simulations on 2D clusters, using VCPT [88, 89] and DCA [13], they are likely not artifacts of our cluster choice, despite its breaking rotational symmetry. The remarkable agreement with other approaches on square clusters indicates that our ladders contain a great deal of information and display features corresponding to the 2D physics of the Hubbard model: features of the ladders at half-filling indicates the onset of long range AFM correlations and the charge excitations start resembling quasi-particle peaks, but the spinons manifest themselves as incoherent background at low energies. In addition, 2D-AFM long-range order exist only at zero temperature, so it is conceivable that most of the CPT spectrum furnishes a faithful representation of the excitations of the system at finite $T$, after the correlation length reduces to a few lattice spacings, as also suggested by the aforementioned QMC results[100].

This study also showed that the combination of tDMRG and CPT can be used as a numerical tool to study the electronic excitations of two-dimensional system with local interactions. Due to the limited capability of computer, some discontinuity seems to be unavoidable, but the results has indeed provided us essential information and this shortcoming in principle can be cured by adding more legs of the ladder to the cluster in the future. Since our approach (CPT) fails to account for the presence of
of long-range antiferromagnetic order in two dimensions, what the fate of spin and charge separation in the presence of long-range antiferromagnetic correlations is, or equivalently how spectral function will be changed in the presence of long-range antiferromagnetic order remains open. So we cannot assume about the spectral function of 2d Hubbard model at zero temperature by simply extrapolating from our calculations. To answer this question, we need further explorations, which include the AFM long-range order explicitly.
Chapter 4

The spectral function of
Mott-insulating Hubbard ladders:
From fractionalized excitations to
coherent quasi-particles

The work presented in this chapter has been submitted to Phys. Rev. B

4.1 Background

It is well known that low energy excitations in one dimensional systems correspond
to the bosonic density excitations–holons and spinons–one carrying the charge but
no spin and the other carrying the spin without charge, rather than the conventional
quasi particles in Fermi liquid theory. This is called “spin-charge separation”, a par-
ticular case of fractionalized excitations in condensed matter physics: An electron
with momentum $k$ “splits” into holons and spinons with momentum $q_h$ and $q_s$, re-
spectively, but momentum conservation requires that $k = q_h + q_s$. As a consequence,
the spectrum is characterized by an incoherent continuum of excitations rather than a coherent band of quasiparticle. A natural question arises when multiple chains get coupled together forming quasi-2D or even 2D systems: What the fate of these density fluctuations is. This question becomes a hot topic and has been extensively debated, particularly within the context of high-temperature cuprate superconductivity, where spinon and holons are conjected to be responsible for the unexpected spectral features such as kinks, and ‘waterfalls’ in cuprates, leading to antiferromagnetic and superconducting phases, respectively. Part of the controversy circles around the interpretation of the pseudogap phase in the cuprates, upon crossing the boundary from the superconducting to the normal state. A dramatic suppression of the quasiparticle weight at the Fermi level in this phase has been verified experimentally and is difficult to understand in terms of a phase transition but might be better interpreted as fractionalization of electrons into charge and spin degrees of freedom in the normal state.

On the theoretical side, much research has been devoted to the study of multiple-leg Fermi Hubbard Hamiltonian or its descendent $t - J$ model, which contain the basic ingredients to understand the physics emerging from strong interaction and low dimensionality. Moreover, their two-dimensional versions have been assumed for decades to be the minimal models to understand high temperature cuprate superconductivity and have been realized recently in ultracold atomic physics. In the previous work of the combination of time-dependent density matrix renormalization group (tDMRG) method and cluster perturbation theory (CPT), we have found that several features associated to spinons and holons survive in the spectral function of the 2D Hubbard model. Since the clusters we exactly solve are very large 2-leg ladders, the calculations are in remarkable agreement with quantum Monte Carlo (QMC), variational cluster approximation (VCA), and dynamic cluster approximation (DCA) on square clusters, indicating that Hubbard ladders contain a great deal of information about the 2D physics: The spectrum shows signatures of both coherent polaron-like quasiparticles and electron fractionalization in terms of spinons and
holons. It is conceivable that the CPT spectrum furnishes a faithful representation of the excitations of the system at finite temperature, since two-dimensional antiferromagnetic long range order exists only at zero temperature and the correlation length reduces to a few lattice spacings at finite temperature, as suggested by the afore-mentioned QMC result.

According to the study of 2-leg Hubbard ladder, it was indicated that both spin and charge degrees of freedom in the Mott insulating phase are gapped, and spins tend to form rung singlets that condense into a “rung-singlet phase”. But once doped with holes, the ladder behaves quite different from a two-dimensional doped antiferromagnet: Upon the introduction of a vacancy by removing an electron, a singlet is broken and the hole will tend to bind with the unpaired fermion and form a polaron that behaves as a quasi-particle. Due to the reflection symmetry of 2-leg ladder, there are two types of polarons corresponding to the symmetric and antisymmetric channels ($k_y = 0, \pi$). Recently, a series of work proposed [107–112] that doping a Mott insulating anisotropic $t - J$ ladder would localize the hole and, as a consequence, the system would not support the conventional quasi-particle picture. By using extensive numerical calculations, White et al. [113] demonstrated that in reality there is no localization but a change in the quasiparticle dispersion, with the minimum of the hole band moving away from $k_x = \pi$ as the ratio $\alpha = \frac{t_x}{t_y}$ changes [114, 115] ($t_x$ and $t_y$ being the hopping along the leg and rung direction of the ladder, respectively). Therefore, doping the Mott insulating ladder would be equivalent to doping a band-insulator, where quasi-particles correspond to renormalized holes that were very robust. Later this picture was confirmed by large scale DMRG studies [116], which further determined the critical value of the anisotropy parameter $\alpha$, at which the quasi-particle mass diverges. Authors argued that in the large $\alpha$ regime, where the chains are weakly coupled, the polaron is an extended object with a complex internal structure in which charge and spin locally behave as separate degrees of freedom.

To shed light on these questions, we carry out time-dependent DMRG simulations
[73] that allow us to obtain spectra with unprecedented resolution. We first present analysis of the results for the excitation spectrum and then study the real-time dynamics of charge and spin by carrying out a “time-of-flight” numerical experiment to identify the nature of the processes leading to quasi particle formation. To understand the spectra, we compare the simulation results with some analytic results from “Random Phase Approximation” (RPA) and “Local Rung Approximation” (LRA) calculation.

4.2 Model and methods

In this work, we consider anisotropic model with hoppings along the legs $t_x$ and along the rungs $t_y$, taking $t_x = 1$ as our unit of energy:

$$H = -t_x \sum_{i,\lambda,\sigma} (c_{i,\lambda\sigma}^\dagger c_{i+1,\lambda\sigma} + h.c.) - t_y \sum_{i,\sigma} (c_{i,1\sigma}^\dagger c_{i,2\sigma} + h.c.) + U \sum_{i,\lambda} n_{i,\lambda\uparrow} n_{i,\lambda\downarrow}$$

where the operator $c_{i,\lambda\sigma}^\dagger$ creates an electron on rung $i$ and leg $\lambda = 1, 2$ with spin $\sigma = \uparrow\downarrow$, $n_{i,\lambda\sigma}$ is the electron local number operator, and $U$ parameterizes the on-site Coulomb repulsion.

In the following, we calculate the photoemission spectrum (PES), which contains information about the one-hole dynamics and is measured by $G^< (x,t) = \langle c^\dagger(x,t) c(x,0) \rangle$, of $2 \times L$ Mott insulating Hubbard ladders with $L = 80$ using the adaptive time-dependent DMRG method. (Due to the particle-hole symmetry, we just focus on the (PES) part). Since Hubbard ladder is gapped in both charge and spin sectors, we used a time step $dt = 0.02$ and up to 800 DMRG states, that for times $t < 40$ translates into a truncation error of the order of $10^{-5}$ or smaller (smaller values of $t_y$ give large error). As previous, a Hann window with $t_{max} = 40$ is adopted to minimize boundary effects and other artifacts such as ringing resulting from the finite size of the lattice and time interval.
4.3 Results

4.3.1 Spectral function

Results for the spectral function are shown in Fig. 4.1, where the color density depicts the spectral weight as a function of momentum $k_x$ and frequency $\omega$. Each column corresponds to different values of $t_y$ and each row to two possible transverse momenta $k_y = 0, \pi$ representing bonding and anti-bonding symmetry sectors with respect to reflections along the leg direction.

![Spectral function of a Hubbard ladder with $L = 80$ and $U/t = 8$, at half-filling, obtained with tDMRG. Top and bottom rows show the symmetric and anti-symmetric sectors, respectively. We only plot the PES part of the spectrum. Notice that the color scale varies from panel to panel.](image)

For small $t_y$, we find clear signatures of spin-charge separation. Curiously, most of the spectral weight on the spinon branch goes to the $k_y = \pi$ sector, while the holon
branches dominate the $k_y = 0$ sector. In Figs.4.1(a) and (e), we clearly observe an avoided level crossing at low energies that indicates hybridization between spin and charge, with the spectral weight accumulating around the Fermi points. This spectral weight corresponds to the polaron (the bound state of spin-hole rung pair), which would not be well-defined at energies larger than $E_0 - J_y$, with $E_0$ the top of the polaronic branch and $J_y \sim \frac{t_y^2}{U}$. In this regime, the hole would move without an associated spin degrees of freedom, same as a holon in 1D chain.

As $t_y$ increases, we can find another avoided level crossing at $k_x = 0$ that merges the two holon branches into a single band with finite curvature. This resembles the spectrum of a single hole in a spin-incoherent Luttinger liquid [117–124], where the vacancy moves in a background of incoherent spins. These results can be compared to those obtained from an RPA treatment of the single chain spectrum.

**Weak coupling**: In an RPA treatment, the interchain hoppings are treated as perturbation, so we obtain a RPA equation

$$G_{RPA}^{-1} = G_0^{-1} - t_y \cos(k_y)$$

where $G_0$ is the exact Green’s function of the 1D Hubbard chain and $k_y = 0, \pi$. The resulting spectral function $A_{RPA}(k_x, \omega) = -\frac{1}{\pi} G_{RPA}(k_x, \omega)$ for $t_y = 0.5$ is shown in Fig.4.2: They can reproduce the dominant holon and spinon branches in the $k_y = 0$ and $\pi$ sectors, respectively. However, it fails to account the bound state–polaron, a genuine quasi two-dimensional feature.

**Strong $t_y$ regime**: The larger $t_y$ regime (Fig.4.1(d) and (h)) is intuitively easier to understand: the Mott insulating ground state is a product of local rung dimers. Upon doping with a single hole leads to the creation of a coherent rung polaron that propagates as plane wave on top of the dimer vacuum. This seems to be equivalent
to introducing a vacancy in a chain of spinless fermions with one particle per site, which is just a band insulator, and leads to a cosine-like dispersion.

However, if we analyze the motion of the polaron carefully, we can find that they cannot move without disrupting the spin background [125], especially for small $t_y$. As a result, their motion requires an effective second neighbor hopping, indicating the minimum of the dispersion should be $k_x = \pi$ if higher order spin flips are ignorable. In practice, the minimum of the hole dispersion can shift away from $k_x = \pi$, as observed in Fig.4.1(b), depending on the parameters of the model.

To seek stronger support for this physical picture, we construct a polaronic variational wave function following [126]. Details can refer to the Appendix. In the so-called “Local Rung Approximation” (LRA), the Mott insulating state $|\psi_0\rangle$ consists of a product of localized singlet rung dimers $|S_i\rangle$, each being the ground state of the local rung Hamiltonian. The excited states are constructed as plane waves with a single polaron, so we can assume two possible values $k_y = 0$ and $\pi$:

$$|\psi_1(k_x, k_y)\rangle = \sum_x e^{ik_xx} |x, k_y\rangle$$
with the state \( |x, k_y \rangle \) being defined as

\[
|x, k_y \rangle = |S_1 \rangle |S_2 \rangle \cdots |k_y \rangle \cdots |s_L \rangle
\]

The dispersion for \( \omega < 0 \) is given by

\[
\omega(k_x, k_y = 0, \pi) \equiv \langle \psi_0 | H | \psi_0 \rangle - \langle \psi_1(k_x, k_y) | H | \psi_1(k_x, k_y) \rangle - \mu
\]

\[
= \begin{cases} 
E_- + t_y - t_x A(0) \cos(k_x) - \frac{U}{2} & k_y = 0 \\
E_- + t_y - t_x A(\pi) \cos(k_x) - U & k_y = \pi
\end{cases}
\]

where \( E_{\pm} = \frac{U}{2} \pm \sqrt{\left(\frac{U}{2}\right)^2 + 4t_y^2} \), \( A(0) = \frac{(1 + \frac{E_+}{2t_y})^2}{1 + (\frac{E_+}{2t_y})^2} \) and \( A(\pi) = \frac{(1 - \frac{E_+}{2t_y})^2}{1 + (\frac{E_+}{2t_y})^2} \).

In Fig.4.3, we reproduce the results for \( t_y = 2 \) in a different color scale to resolve fainter features in the spectrum. We first observe that the coherent band in the bonding sector is perfectly described by the LRA, as previously reported in QMC calculations [126]. However, in the \( k_y = \pi \) channel, the LRA yields energies slightly lower, while correctly describing the corrections to the bandwidth. The smaller
bandwidth results from cancellations due to the symmetry of the wave-function and the fermionic sign that introduce destructive interference preventing processes that do not conserve double occupation. This also translates into a much smaller spectral weight in this band, which makes it difficult to resolve with other numerical methods.

**Scattering states of triplon and polarons**: In addition to these two types of polarons, our tDMRG calculations allow us to identify a continuum at energies centered around $-10t_x$, near the bottom of the bonding band and another continuum of excitations at low energies of the order of $-5t_x$ in the anti-bonding sector. The high intensity peak at low energies near $-4t_x$ in Fig.4.3(b) corresponds to the edge of a two-particle continuum.

Obviously, these continuum should correspond to scattering states of triplon, which can assume three possible polarizations $|\uparrow_1\uparrow_2\rangle$, $|\downarrow_1\downarrow_2\rangle$ and $\frac{1}{\sqrt{2}}(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)$, and polarons with different spin polarizations. In general, their scattering resultants involve two independent “spin” channels: $S = \frac{3}{2}$ and $S = \frac{1}{2}$. As discussed in [127, 128], the spin $S = \frac{3}{2}$ has higher energy than the bottom of the polaron, so it’s unstable and only exists as a resonance during the triplon-polaron scattering, in accordance with Nagaoka’s theorem in our parameter regimes. This is consistent with the above spectral function in Fig.4.3(a) where its decay width is rather broad and the scattering state has higher energy than the polaron.

In the symmetric sector, we attribute the high energy states to the triplon and an anti-bonding polaron, while in the anti-symmetric sector, to a triplon and a bonding polaron. As an evidence, we can calculate the zeroth order energies of these states within the LRA

$$\omega_{\pm} = 2E_- - \frac{U}{2} \mp t_y$$
which are plotted in the Fig.4.3. The high-order corrections can disperse the spectral weights but the center remains unchanged, so we can find the the scattering states of a triplon and a symmetric polaron live in the anti-symmetric sector and vice-versa. In the weak coupling case, the scattering continuum for \( k_y = 0 \) overlaps with the polaron band. As the interchain hopping increases, the continuum moves to higher energies and the dispersion becomes more coherent. Similar effect occurs in the \( k_y = \pi \) sector, with the scattering continuum shifting to lower energies.

### 4.3.2 Real-time dynamics

To confirm this picture, we can carry out a “time-of-flight” numerical experiment by creating a vacancy at the center of the ladder and observing the propagation of the hole density \( \langle n(x, t) \rangle \) and spin \( \langle S^z(x, t) \rangle \) fluctuations, as shown in Fig.4.4. For simplicity, we just show results for one of the legs where the vacancy is created. We can notice nodes along the \( x \) direction that results from the density alternating between legs. In 1D chains, one can observe \([129–132]\) two lightcones of excitations propagating coherently with maximum velocity \( v_s \) and \( v_c \) for spin and charge, respectively. Similar features present on panels Fig.4.4(a) and (e) corresponding to small \( t_y = 0 \) as well: At short times, there are two lightcones that propagate with the characteristic spin and charge velocities. However, the emitted holons fade away rapidly, with the wavepacket spreading over the entire volume and losing coherence, while the spinons remain coherent up to the largest simulated time. At longer times \( t \sim 15 \), we can identify the emergence of two clearly defined branches in panel (a) that have the same slop as the spinons. Now the picture becomes clearer: after injecting a vacancy, incoherent holons and spinons are emitted, but after a characteristic time \( \tau \sim \frac{1}{t_y} \) a polaron is formed, that propagates with a velocity \( v_c \sim v_s \).

As \( t_y \) is increased, holons become heavier, and for large \( t_y \), polarons are the only type of excitation that remains observable. In this case we can see two dominant branches corresponding to the maximum velocities for the \( k_y = 0 \) and \( k_y = \pi \)

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Figure 4.4: Top panels display the time evolution of charge density after a hole is injected at the center of one of the leg. Similar results for the spin density are plotted in the bottom panels. Here we only show data for the leg on which the hole is created.

coherent bands. Interestingly, for $t_y = 1.5$ we find a clear and bright mode that seems localized: This is due to the tiny curvature of the dispersion for $k_x = 0$, which becomes practically flat. In fact, it was shown that the effective mass diverges at the value of $1/\alpha = t_y/\tilde{t}_y \sim 1.4$ for $U/t = 8$ [113, 116]. This type of localization should not be attributed to a breakdown of the Fermi-liquid picture [107–112].

Cross correlation functions: To measure the coherence between spin and charge degrees of freedom, we analyze the cross correlation between the two datasets:
For each time slice, we calculate the quantity

$$C(t) = \frac{\sum_x \langle n_1(x, t) \rangle | \langle S_z(x, t) \rangle |}{\sqrt{\sum_x \langle n_1(x, t) \rangle^2} \sqrt{\sum_x \langle S_z(x, t) \rangle^2}}$$

which is equivalent to the overlap between two normalized vectors, one with component defined by the density on one leg $\langle n_1(x, t) \rangle$ and the other, by the spin on the another leg of the ladder, $|S_z(x, t)|$. If these two quantities are perfectly correlated, $C = 1$. Results for the cross correlation are displayed in Fig.4.5 for different values of $t_y$.

![Figure 4.5: Cross correlation between spin and charge density as a function of time, for different values of $t_y$. In panel (a), we include the results for a single chain with $U = 8$ for comparison.](image)

In the Mott insulating regime for $t_y = 0.5, 1$, we observe rapid oscillations preceding a quasi-steady behavior. Such transient can be associated to the time scale required for the formation of polaron. In the band insulating regime for $t_y = 1.5, 2$, the behavior is actually more complex due to the presence of two clearly distinct lightcones corresponding to the $k_y = 0$ and $\pi$ channels that produce a great deal of
interference, which is enhanced by the rapid oscillations of the hole along the rung in the transverse direction region. In this case, spin and charge are quite correlated but most of the overlap is concentrated in the \( k_y = 0 \) sector that contributes with the greater weight. Ideally one would like to resolve and compare their contributions separately, that should therefore be normalized independently. Since there is no obvious way to do this, we find that the overall correlation is actually reduced. For \( t_y = 2 \), we are no longer able to clearly distinguish a transient, although we can identify a dip that is associated to the wave packets bouncing off the edges of the ladder. Interestingly, although we cannot assert this clarity, for weak interchain coupling we see indication that \( \tau \) and, consequently, the polaron binding energy do not depend strongly on \( t_y \) and (at least in the Mott insulating regime and for this value of \( U \)) is of the order of \( \tau \sim 20 \). This time seems considerably reduced after the system undergoes a crossover to the band insulting regime.

4.4 Conclusion

In this chapter, we adopted the tDMRG to simulate the anisotropic Hubbard ladder. Our simulations offer a new perspective on the physics of Hubbard ladders enabling us to resolve fine details of the spectrum with unprecedented resolution. Among some of the main features we highlight the appearance of avoided level crossings at weak interchain indicating hybridization between spin and charge, although most of the main features of the spectrum can still be traced back to the physics of one-dimensional chains. Moreover, we find that the excitation spectrum is dominated by multi-particle states. Coherent polarons emerge from this continua as spin \( S = \frac{1}{2} \) and charge \( e \) quasi particles, a bound state of a holon and a spinon: Symmetric \( k_y = 0 \) polarons can propagate coherently through first order processes and become the relevant excitations in the large \( t_y \) regime, while anti-symmetric polarons become heavier and lose spectral weight due to the symmetry of its wavefunction and fermionic sign. The most relevant scattering states consists of a triplon and a
polaron assuming different spin polarizations: The symmetric (anti-symmetric) polarons are responsible for the continuum in the $k_y = \pi(0)$ sector, and the coherent quasi-particles emerge from these continua, as the scattering states shift to lower (higher) energies.

In the antisymmetric channel, the continuum of scattering states has a sharp edge at low energies that consists of bound states with spin $S = \frac{3}{2}$. The formation of bound states with higher spin near the $(0,\pi)$ point implies that “spin bags” might be realized in the two-dimensional counterpart between the $X$ and $M$ points of the Brillouin zone. These excitations would have a short lifetime and decay into a triplon and a polaron, respectively. This is an manifestation of the Nagaoka mechanism in which a hole surrounds itself by ferromagnetic cloud to propagate more efficiently.

In order for the spin polaron to behave as coherent quasi-particle, the system size has to be considerably larger than the characteristic size $\lambda$ of the polaron. If $\lambda$ is of the order or larger than the system size, the above numerical results would not be able to resolve the quasi-particle and would mistakenly lead one to conclusion that quasi-particles are not stable objects.
Chapter 5

Excitonic density waves, biexcitons and orbital-selective pairing in two-orbital correlated chains

The work presented in this chapter has been published in Phys. Rev. B 98, 035128 (2018).

5.1 Background

Viable optoelectronic device [133–135] usually involves the process of photoinduced charge transfer and charge recombination. Recently, its construction is based on organic semiconducting devices due to the band edge singularities, that could give rise to a high-differential optical gain, in one-dimensional (1D) materials such as conjugated polymers [136]. Such materials have already found uses in a wide range
of applications such as light-emitting diodes, lasers, sensors, and molecular switches [134, 137–143].

Physically, the bound state of electron-hole pairs, known as excitons, plays a vital role in such optoelectronic devices. These neutral particles and their condensation have been studied in different contexts and systems (as shown in Fig. 5.2) in condensed matter physics. In semiconductor, they are slightly bound, called the Wannier-Mott excitons, and their condensation opens the charge gap [144–147]. In strongly correlated systems, there are different types of excitons, such as Frenkel excitons, Mott-Hubbard excitons, and the recently proposed Hund excitons [148, 149], which are more tightly bound objects.

As a matter of fact, excitons in low-dimensional strongly correlated electronic materials have received much theoretical attention [150–156], especially in the context of High-$T_c$ cuprates, iron pnictides, manganites, and transition-metal oxides, and they have also been observed experimentally in one-dimensional (1D) Mott insulators [156, 157], where the low energy excitations are bosonic density fluctuations,
called *spinon* and *holon*. These excitations propagate independently, called spin-charge separation. In multiorbital systems, excitonic instabilities typically have been studied in pump-probe spectroscopy, which aimed at unveiling the complex interplay between charge, spin and orbital degrees of freedom [157, 158] and how these bosonic excitations decay. On the theoretical side, most studies focused on single-band Mott physics, such as the excitons formed by the doublon and holon in extended Hubbard model. Early studies in multiband Mott insulators indicated that the excitation of orbitals, known as orbitons, may also decouple from the spin in what is referred to as “spin-orbital” separation. This phenomena can be understood by starting with the simplest model describing a Mott insulator and accounting for both spin and orbital degrees of freedom, the Kugel-Khomskii chain [159]. It has been shown that the problem of a propagating orbiton can be mapped onto the dynamics of a hole in an antiferromagnet [157, 160–163], leading to an effective $t - J$ model, which is much simpler and has been extensively studied in the literature. In one dimension, the physics is described in terms of LL theory, which naturally explains spin-orbital separation. In addition to the excitons, multiorbital systems can contain Mott and Hund physics, and are rich in various phenomena, including orbital selective Mott transitions [164–167], spin-orbital separations [157, 160–163], spin-incoherent behavior [168, 169] and pairing density wave [170–172]. Therefore, it captures many unique features in real strongly correlated systems, such as iron pnictides and ruthenates, and thus deserves more careful investigations.

In the following, we will study a two band problem in the limit of weak Hund coupling and inter-orbital hopping, and strong Coulomb repulsion. In this regime, we can assume a two orbital model described by two $t - J$ chains coupled electrostatically via an inter-orbital Coulomb repulsion $U'$. As a zeroth order approximation, we ignore inter-orbital hopping, meaning that the number of particles is separately conserved for each orbital type. In addition to spin and orbital degrees of freedom, this model accounts for charge fluctuations and can be considered as an extension of the Kugel-Khomskii model with charge fluctuations. Using analytical and density
matrix renormalization group techniques (DMRG) [69, 70, 173], we study its phase diagrams and the associated correlations in various phases. Based on the analytical results, we expected to provide unique insight into the behavior of the system and offer an intuitive picture of the mechanism leading to the observed phases.

5.2 Two orbital $t - J$ Model

The modified two orbital $t - J$ model is described by the Hamiltonian

$$H = -t \sum_{i, \sigma, \lambda} (c_{i \sigma \lambda}^\dagger c_{i+1, \sigma \lambda} + H.c.) + J \sum_{i, \lambda} (\vec{S}_i \cdot \vec{S}_{i+1, \lambda} - \frac{1}{4} n_{i, \lambda} n_{i+1, \lambda})$$

$$+ U' \sum_i n_{i1} n_{i2} + \Delta \sum_i (n_{i1} - n_{i2})$$

where $c_{i, \sigma, \lambda}^\dagger$ is a fermionic creation operator acting on site $i$ and orbital $\lambda$ ($\lambda = 1, 2$) with spin $\sigma = \uparrow, \downarrow$, and the constraint forbidding double occupancy is implicit as usual. The operators $n_{i, \lambda}$ represent the local density, and $\vec{S}_i$ refer to the local spin. Here the hopping along the two legs $t$ are taken to be equal for simplicity and to be the unit of energy. The coupling between two chains are characterized by the on-site interorbital Coulomb repulsion parameterized by $U'$ and the crystal-field splitting $\Delta$. Compared to the conventional multi-orbital Hubbard model, we have ignored the Hund coupling and interorbital hopping, since, for instance, in $Sr_2CuO_3$ the Hund coupling is one order of magnitude smaller than the on-site Coulomb repulsion [174]. By analogy, this model can also represent strongly interacting electrons on two parallel chains coupled via an electrostatic Coulomb repulsion.

We will consider the total number of electrons to be constant, then the crystal-field splitting $\Delta$ determines the relative population of the two bands in the ground state. For large $\Delta$, the model will display an indirect gap. Clearly, the total spin $S^z$, the number of electrons $N$ and their components on each orbital chain are conserved. This means that $N_2 = N - N_1$ remains constant and the last term of the Hamiltonian
becomes just a constant shift

\[ \Delta \sum_i (n_{i1} - n_{i2}) = \Delta (2N_1 - N) \]

which means that the crystal-field splitting basically plays the role of a chemical potential for orbital excitations. That is, the number of particle-hole pairs in the ground state could be arbitrarily tuned by changing \( \Delta \). (If interorbital hopping is taken into account, photoinduced excitations can be created to adjust the number of particle-hole pairs). Obviously, when \( \Delta > 2t \), \( N_2 \) vanishes, i.e. all electrons occupy the lower band. Regardless, one could fix \( N_1 \) and \( N_2 \) independently. Particularly, the case \( N_1 = N_2 = L \) describes two independent Heisenberg chains without charge fluctuations. In the following we focus on the case \( N \leq L \) or density below quarter filling.

### 5.2.1 Some particular cases

Before any analytic or numerical calculations, we can gain some basic intuition into the problem by looking at particular cases.

First, we consider \( J = \Delta = 0 \). In the absence of spin interactions, the spin degree of freedom becomes spurious and only charge and orbital degrees of freedom are involved. We can map each orbital onto a pseudospin quantum number and identify \( \lambda = 1(2) \rightarrow \sigma = \uparrow (\downarrow) \). The problem is now equivalent to a one-dimensional single-band Hubbard model with \( U' \rightarrow U \) and a magnetic field \( 2\Delta \), which has been extensively studied. This can help us understand what happens in this limit. If \( \Delta = 0 \), quarter filling corresponds to half filling, and the ground state becomes an unpolarized Mott insulator with vanishing spin gap but finite charge gap. By analogy, creating an exciton by applying \( c_{2\uparrow}^\dagger c_{1\downarrow} \) can be understood as \( S^+ = c_{1\uparrow}^\dagger c_{1\downarrow} \), so no spin gap indicates that excitons can be created freely without paying any energy. But finite charge gap can be associated with the binding energy that holds the exciton together, since it costs energy of the order of \( U' \) for an up particle to hop to
a neighboring site already occupied by a down particle. Moreover, the short-ranged anti-ferromagnetism in the ground of Hubbard chain would translate into short-ranged orbital order in the original two-orbital problem, which indicates biexcitons don’t form in this limit, since biexciton would imply ferromagnetic correlations in the Hubbard chain. However, away from quarter filling the presence of empty sites allows the up particles to hop. In this situation, both spin and charge sectors become gapless and therefore the system becomes a Luttinger liquid, meaning that particles and holes can freely move. If we introduce $J$, this mapping is no longer valid.

A second limit corresponds to $U' = 0$. This maps onto two decoupled $t - J$ chains, whose ground state has been extensively studied [4] as well. In this situation, excitons become unstable quasiparticles. For large $\frac{J}{t} > 2$ and intermediate densities, the ground state presents dominant pair-pair correlations that decay algebraically, indicating the formation of a quasicondensate of superconductivity, which has to be distinguished from an excitonic quasicondensate. Therefore, by introducing a crystal-field splitting, it is possible that two orbitals realize different phases: One band can realize pairing, while the other one remains a metal.

Finally, for finite $J$, large $U'$ and $\Delta$ at quarter filling, a single exciton is strongly bound and the particle-hole pair can move coherently through high-order processes. This scenario can be identified with the motion of a single hole in an antiferromagnetic background [161]. However, the case at finite exciton density needs a deep description, which is still lacking.

### 5.3 The Electron-Hole-Spinon Problem

Now we consider special cases where analytic calculations are available. They can provide us some intuitive guidance.
5.3.1 Single Exciton

To develop some insight into the nature of the exciton condensate in this model, we study a toy problem of one single exciton in the Ising limit, i.e. in the limit of strong uni-axial anisotropy [22, 175–180]. We focus on the system at quarter filling and with the crystal splitting $2\Delta$ larger than the bandwidth $4t$. In this situation, the system has one electron per site and the lower band is half filled but the upper band is empty. As a result, the ground state of the system is just an Ising antiferromagnet. If we create an electron by promoting an electron to the upper band, a hole in the lower band is left out. Since interband hopping is ignored, it will never decay back to the lower band. It is intuitive to guess that the Coulomb repulsion $U'$ acts as an on-site attractive potential between the electron and the hole, and thereby yielding a bound state of the particle-hole pair. In the following we will analyze the formation of this bound state. For a two-particle bound state in Hubbard-like models, the studies have been done in a number of setups in the literature [181–189]. However, in our scenario, the situation becomes more complicated, since the motion of the hole will leave behind a misaligned spin, a domain wall or spinon, which costs an energy $J$. The presence of this defect makes it become a three-body problem in one-dimension. As complicated as it may sound, it turns out to be tractable approximately as follows. We can choose a basis of states characterized by the position of the electron $r_e$, the position of the hole relative to the electron $r = r_h - r_e$, and the position of the domain wall relative to the position of the hole $r_s = r_w - r_h$, as illustrated in Fig.(5.2):

\[
H|r_e, r, r_s\rangle = -t(|r_e + 1, r - 1, r_s\rangle + |r_e - 1, r + 1, r_s\rangle + |r_e, r + 1, r_s - 1\rangle + |r_e, r - 1, r_s + 1\rangle) \\
+ U'|\delta_{r\neq 0}|r_e, r, r_s\rangle - J\delta_{r_s, -1}|r_e, r, r_s\rangle + J(|r_e, r, r_s + 2\rangle + |r_e, r, r_s - 2\rangle) \tag{5.1}
\]
where we assume periodic boundary conditions. We can construct a basis of states that preserve translational invariance and are labeled by a momentum \( k \):

\[
|k, r, r_s\rangle = \frac{1}{\sqrt{L}} \sum_{r_e=1}^{L} e^{ikr_e} |r_e, r, r_s\rangle
\]

and obtain the matrix elements of the Hamiltonian, which can be diagonalized numerically for very large chains.

In the \( J = 0 \) limit, we should recover the results for two particles without a spinon and observe a band of bound states with a minimum at \( k = 0 \) for sufficiently large \( U' \). (This is consistent with our intuition that if the binding energy is smaller than the kinetic nenergy of a free electron and hole, we will not obtain bound states.) After introducing \( J \), the bound state behaves as a hole in the antiferromagnet that propagates coherently. If \( J \) is sufficiently large, the free spinon can bound with the electron-hole pair, forming a three-body bound state, where the domain wall will be “absorbed” by the electron-hole pair bound state. In order to account for the spin fluctuations, we take the assumption used in the seminal paper by Villain [190]: we consider only spin-flip processes that move the domain wall and ignore those that create new ones because they are energetically not favable. It is easy to see that the spinon can propagate by two sites for each spin flip, and therefore, it has a dispersion.
\( \epsilon_s(k) = 2J \cos(2k) \). When it binds with the particle-hole pair, the larger mass of spinon will tend to localize the particle-hole pair, giving it a quite flat dispersion. However, this bound state can still move as a whole, as shown in Fig.(5.3).

![Figure 5.3](image)

**Figure 5.3:** Cartoon describing the high-order effective hopping of an exciton-spinon bound state. Each spin flip shifts the spinon by two lattice spaces. The exciton moves to remove the magnetic domain wall but binds with the spinon as a single object.

In order for this to happen, the bound state has to hop by two lattice spaces accompanied by a spin flip, such that the resulting motion does not disrupt the antiferromagnetic background. Effectively, this spinon-exciton object can propagate with an effective second-neighbor hopping, leading to a minimum in the dispersion at \( k = \pm \frac{\pi}{2} \) and a maximum at \( k = 0 \).

![Figure 5.4](image)

**Figure 5.4:** Excitation energies for the electron-hole-spinon problem. The lowest-energy band has a double-dip dispersion with minima at \( k = \pm \frac{\pi}{2} \). The system size is \( L = 40 \), and we used \( U' = 8, J = 6 \) to enhance the main features.

As a hint of what it means, we can consider the system with a finite density of excitons. Since excitons as a whole behave like bosons, they can condense with
momentum $k = \pm \frac{\pi}{2}$ and thereby can break the $Z_2$ symmetry by choosing one of the two momenta, or more likely, can form an equal superposition, corresponding to an order parameter that would oscillate in real space as $\Delta_{\text{cond}} \sim \cos(\frac{\pi x}{2})$. Notice that the spinon-exciton bound state involves both spin and orbital degrees of freedom. But we should keep in mind that this picture assumes a classical magnetic ordering, which might be destroyed by quantum fluctuations in lower dimensional systems. In the isotropic $SU(2)$ limit, the spinon forms a deconfined excitation and propagates independently, giving rise to the spin-orbital separation picture.

5.3.2 Biexcitons and Phase segregation

A low density of excitons corresponds to a low density of electrons in the upper band. According to the phase diagram of the 1D $t - J$ chain [4], for sufficiently large value of $J$ and at low densities the ground state of the model becomes superconducting with a quasicondensate of singlets held together by a binding energy of the order of $J$. In our model, such pairs can be formed by excitons: that is, electrons can form spin singlets by an energy of $J$ in both upper and lower bands and those in the upper band correspond to the biexcitons. Therefore, it is expected that for moderate values of $J \sim t$ the system will realize a quasi-condensate of biexcitons. It does not prevent the formation of excitonic “strings”, where the excitons clump together, forming a separate domain. This would give rise to phase segregation and correspond to a region of instability in the phase diagram where the excitons and conduction electrons are spatially separated: electrons on each band will form a string coupled only via the Heisenberg exchange term $J$ and will occupy distinct regions of space, hence behaving as two independent Heisenberg chains. This occurs when $U'$ is large and excitons become very heavy.
5.4 Numerical results

We conduct DMRG calculations for chains up to $L = 64$ with open boundary conditions while keeping the truncation error below $10^{-6}$, which requires of the order of 2000 states in some cases. Most results, unless otherwise stated, correspond to $L = 64, N_1 = 48$ and $N_2 = 16$, with Fermi momenta $k_{F_1} = \frac{3\pi}{8}$ and $k_{F_2} = \frac{\pi}{8}$, respectively.

5.4.1 Ground state

We first analyze $N_1$ vs. $\Delta$ for different values of the interaction $U'$ and $J$, as shown in Fig.(5.5)

![Figure 5.5: Ground-state occupation $N_1$ of the first orbital chain as a function of the band splitting $\Delta$ for a chain of length $L = 32$. The total density is quarter filling, and the occupation of the second chain is given by $N_2 = L - N_1$. Results for (a) $J = 0.6$ and (b) $J = 1$ for several values of $U'$. The biexciton instability is signaled by jumps in steps of two.](image)

In the simulation, we fixed the values of $N_1$ and obtained the curves by carrying out a Maxwell construction. For small values of $J$ and $U'$, the curves show a smooth behavior, with the particle number changing in discrete steps of one at a time. However, for densities close to $\frac{N_1}{L} = 1$ or 0 and especially when $J$ is increased, we find that in certain density regimes the jumps are now in steps of two, indicating a pairing instability corresponding to the formation of biexcitons. In order to determine whether these biexcitons are stable objects in the thermodynamic limit, we need
to carry out a finite-size analysis of the binding energies. To distinguish different regimes we first define the binding energy for two particles pairing on each orbital chain separately as

\[
\Delta_{\lambda=1} = [E(N_1 - 2, N_2) - E(N_1, N_2)] - 2[E(N_1 - 1, N_2) - E(N_1, N_2)] \\
= E(N_1, N_2) + E(N_1 - 2, N_2) - 2E(N_1 - 1, N_2)
\] (5.3)

with a similar expression for \( \lambda = 2 \) obtained by exchanging the labels. Obviously, these quantities indicate the binding energy, which is negative in the case of an attraction between particles. This idea can be generalized to the case of a particle-hole pair: the binding energy for the formation of a single exciton is given by

\[
\Delta_{ex} = E(N_1, N_2) - E(N_1 - 1, N_2) - E(N_1, N_2 + 1) + E(N_1 - 1, N_2 + 1)
\]

Results for several parameter regimes and system sizes are shown in Fig.5.6(a), focusing on the regime \( \frac{N_1}{L} = 0.75 \). In Fig.5.6(b), we plot the values in the thermodynamic limit, as obtained from a quadratic fit in \( \frac{1}{L} \). For small values of \( U' \), it is difficult to tell whether the particle-hole excitons form bound states from the results. It is also possible that the electrons in the upper band form bound singlets that propagate independently, as observed in the 1D \( t - J \) chain. However, for large values of \( J \sim 2t \), this would occur. On the other hand, if the value of \( U' \) increases further, the excitons can become very heavy and clump together, so the system phase segregates.

### 5.4.2 Excitonic density waves and charge order

In order to determine the ground-state properties, we study several correlation functions, paying particular attention to the cases with \( J = 1.2 \).
Momentum distribution function (MDF) : It is clear beforehand that the actual excitonic wave function may actually spread over several lattice spaces. Here we just want to describe the underlying ground state and its pairing tendencies. For simplicity, we assume that the excitons are local objects that can be described in terms of bosonic operators

\[ b_{x\sigma}^\dagger = c_{x\sigma}^\dagger c_{x\sigma} \]

, so the biexcitons as exciton pairs can be described in terms of [191, 192]

\[ \Delta_x^\dagger = \frac{1}{\sqrt{2}} (b_{x\uparrow}^\dagger b_{x+1\downarrow}^\dagger - b_{x\downarrow}^\dagger b_{x+1\uparrow}^\dagger) \]

. In terms of these operators, we can introduce the momentum distribution functions of exciton and biexciton, defined as

\[ N_{ex}(k, \sigma, \sigma') = \frac{1}{L} \sum_{x,y} e^{ik(x-y)} \langle b_{x\sigma}^\dagger b_{y\sigma'} \rangle \]

\[ N_{2ex}(k) = \frac{1}{L} \sum_{x,y} e^{ik(x-y)} \langle \Delta_x^\dagger \Delta_y \rangle \]
Since our model does not take into account interorbital hybridization or Hund’s coupling, $N_{ex}$ is always diagonal in the spin index, and from now on we consider only $N_{ex}(k, \uparrow, \uparrow)$ [193].

Figure 5.7: Single-exciton momentum distribution function (MDF) for $L = 64, N_1 = 48, N_2 = 16$, and (a) $J = 1.2, U' = 2$ in the excitonic phase and (b) $J = 1.2, U' = 4$ in the excitonic phase. (c) and (d) the biexciton MDF for the same parameters, respectively.

As shown in Fig.5.7, the excitonic MDF shows a clear peak at $k = \frac{\pi}{2}$, indicating that the quasicondensate of excitons has a finite center-of-mass momentum, an excitonic density wave (EDW), as anticipated. Furthermore, the peaks become more pronounced as $U'$ increases. The biexcitonic MDF shows some structure for $U' = 2$, but the maximum at $k = \pi$ cannot be characterized as a peak, particularly by looking at the scale on the $y$ axis. On the other hand, the one for $U' = 4$ shows a quite dramatic peak, which can be interpreted as a quasicondensate of biexcitons with finite center-of-mass momentum $Q = \pi$ formed by single-exciton pairs with momentum $\frac{\pi}{2}$. This also gives rise to a small peak at zero momentum, but it is less defined and much broader.
Natural orbitals (NOs): We can also study the quasicondensate wave function by means of Penrose and Onsager’s description of the superfluid order parameter [194], the natural orbitals (NOs) $\psi_\alpha$ of the system. The NO with the largest eigenvalue, $\psi_0$, is the single-particle state in which quasicondensate takes place. We generalize this concept to the case of excitons and biexciton: They are simply the single-particle eigenstates, in the bosonic sense, of the bosonic single-particle density matrix

$$G_{ex}(x, y) = \langle b_{x\uparrow}^\dagger b_{y\uparrow} \rangle \quad G_{2ex}(x, y) = \langle \Delta_{x\uparrow}^\dagger \Delta_{y\uparrow} \rangle$$

The results for $U' = 2$ in the excitonic phase and $U' = 4$ in the biexcitonic phase are shown in Fig.5.8.

![Figure 5.8](image)

**Figure 5.8:** Natural orbitals for the exciton condensate with $L = 64, N_1 = 48, N_2 = 16$ in two parameter regimes: (a) $J = 0.6, U' = 2$ corresponding to the excitonic phase, and (b) $J = 1.2, U' = 2$ in the biexcitonic phase. (c) The natural orbital for the biexcitonic condensate. We also show the local occupation of the two orbitals $n_1$ and $n_2$.

The periodicity of the wave function is determined by the characteristic momentum of the condensate: $Q = k_{F_1} + k_{F_2} = \frac{\pi}{2}$ and $Q = \pi$ for single excitons and biexcitons, respectively (see Fig.5.7).
Structure factors: It is important to point out that a quasicondensate with periodicity \( \frac{\pi}{2} \) does not indicate charge order with order \( \frac{\pi}{2} \) (i.e. 1-1-0-0). This would only occur at quarter filling with \( N_1 = N_2 = \frac{L}{2} \). As a matter of fact, the density of excitons is not commensurate with this order. This can be illustrated in Fig.5.9(a) and Fig.5.9(b) by the result for the density-density structure factor:

\[
D_{\lambda}(k) = \frac{1}{L} \sum_{x,y} e^{ik(x-y)} \langle n_{x\lambda} n_{y\lambda} \rangle
\]

\[
D_{ex}(k) = \frac{1}{L} \sum_{x,y} e^{ik(x-y)} \langle n_{ex,x} n_{ex,y} \rangle
\]

where \( n_{x\lambda} = \sum_{\sigma} c_{x\sigma\lambda}^\dagger c_{x\sigma\lambda} \) and \( n_{ex,x} = b_{x,\uparrow}^\dagger b_{x,\uparrow} \) are the number operator for electrons and excitons, respectively. The excitonic structure factor and the one for orbital \( \lambda = 2 \) are practically indistinguishable, indicating that holes and electrons are forming
tightly bound pairs. Signatures of charge order would be identified as peaks at finite momentum: The case $U' = 2$ does not show any such structure and is practically featureless, as expected from a dilute condensate of hard-core bosons/excitons. On the other hand, for $U' = 4$ one can clearly see the onset of charge order with momentum $2k_{F_2} = \frac{\pi}{4}$. It resembles a state in which EDW and charge-density-wave (CDW) orders coexist and are intertwined. But this is not true. In order to determine if this state is a CDW, we calculate the charge gap for adding/removing pairs of excitons, which is defined as

$$\Delta_{ch} = E(N_1 + 2, N_2 - 2) + E(N_1 - 2, N_2 + 2) - 2E(N_1, N_2)$$

(5.4)

A finite-size scaling indicates that this quantity vanishes in the thermodynamic limit, indicating that this state is not quite a CDW, but a quasicondensate of biexcitons, and the modulation observed in the charge density (Fig.5.8) corresponds to slowing decaying Friedel oscillations due to the open boundaries, as also observed in $t-J$ ladders [195]. This conclusion is also consistent with the observation in Fig.5.5: A CDW would be reflected as plateau, which clearly are not present. For completeness, we also show the spin structure factor:

$$S_{\lambda}(k) = \frac{1}{L} \sum_{x,y} e^{ik(x-y)} \langle S_{z_{x,\lambda}} S_{z_{y,\lambda}} \rangle$$

(5.5)

in Fig.5.9. For $U' = 2$, both orbitals display small peaks at $k = 2k_{F_\lambda}$. However, in the biexcitonic phase the peak of orbital $\lambda = 1$ has moved to $k = \pi$, while the structure factor for the orbital $\lambda = 2$ is now completely featureless. This is expected from excitons bound into spin-singlet pairs with short-range correlations. In addition, the peak at $\pi$ indicates that the biexcitons do not disrupt the antiferromagnetic order.
5.4.3 Orbital-selective pairing

Our model can naturally realize an orbital-selective paired phase in which one of the orbitals behaves as a Luttinger liquid, while another orbital undergoes a pairing instability. For small $U'$, the orbitals are practically decoupled and the model behaves like two independent $t - J$ chains. Given relatively large value of $J \sim 2t$, it has been shown that the $t - J$ chain presents a singlet-superconducting phase with a spin gap [4] for lower density $n \leq 0.5$, but realizes a metallic phase for larger density $n \geq 0.5$. Therefore, one can tune the parameter $\Delta$ in our model such that the occupation of each orbital falls into a different phase. This occurs, for instance, for $U' = 0.5, J = 2.4, \frac{N_1}{L} = 0.75, \frac{N_2}{L} = 0.25$. In Fig.(5.10), we show the single-particle binding energy $\Delta E$ for each orbital and the exciton binding energy $\Delta E_{ex}$. The binding energy $\Delta E$ for the low-density orbital is negative indicating pairing, while it remains positive for the high-density one, as expected. In addition, the binding energy for exciton formation is also positive, which is consistent with the assumption that these two orbital chains are effectively decoupled for small $U'$.

**Figure 5.10:** Finite-size scaling of the (a) single-particle binding energy for each orbital chain and (b) exciton binding energy. Results are for $J = 1.2, U'' = 1$ and density $\frac{N_1}{L} = 0.75$.

Due to the number of free parameters in our model $(N_1, U', J)$, determining a general phase diagram would be a tremendous task. Instead, we can show a schematic phase
diagram for the fixed density of interest \( \frac{N_1}{L} = \frac{3}{4} \) in Fig. 5.11 as a function of the interaction \( U' \) and \( J \)

**Figure 5.11:** Schematic phase diagram of the two-orbital model as a function \( U' \) and \( J \) for fixed densities \( \frac{N_1}{L} = \frac{3}{4}, \frac{N_2}{L} = \frac{1}{4} \). Along the \( U' = 0 \) line the system consists of two copies of a \( t - J \) chain at different densities. Finite values of \( U' \) induce the formation of an exciton density wave (EDW), and increasing \( J \) drives an instability toward pairing of excitons (biexciton condensate). At small values of \( U' \) and large values of \( J \) we find the orbital-selective paired phase (OSP).

### 5.4.4 Away from quarter filling

The excitonic physics discussed for the quarter-filling case extends to other filling fractions as well. We show some typical results that we obtained for small densities in Fig. 5.12.

As shown in panel (a), the exciton MDF is peaked at a finite value of \( Q = k_{F_1} + k_{F_2} = \pm \frac{5\pi}{16} \), which is reflected in the behavior of the natural orbitals, displayed in panel (b). The charge structure factor indicates that it is a state with no charge order. In our exploration of parameter space, no bi-excitonic physics has been found, but it may appear at larger values of \( J \) than we expected.
Figure 5.12: (a). Excitonic momentum distribution function for \( L = 64, N_1 = 24, N_2 = 16, J = 1.2 \) and \( U' = 2 \). (b). Natural orbital for the exciton condensate and the local occupation of the two orbitals, \( n_1 \) and \( n_2 \), as in Fig. 5.8. The edge effects are due to the open boundary conditions.

5.5 Conclusion

In this chapter, we proposed a one-dimensional two-orbital \( t - J \) model and comprehensively studied its possible realizations of a number of unconventional phases at and below quarter filling, particularly focusing on the exciton and bi-exciton formation. Physically, the stability of the excitons is determined by the strength of the inter-orbital Coulomb interaction \( U' \), while the formation of bi-excitons is controlled by the antiferromagnetic exchange \( J \). So we provide a schematic phase diagram for fixed densities \( \frac{N_1}{L} = \frac{3}{4}, \frac{N_2}{L} = \frac{1}{4} \) shown in Fig. 5.11. For weak \( U' \), the system behaves as two independent \( t - J \) chains. It is possible that the system is inherently unstable to exciton formation for any finite \( U' \). This would correspond to an exciton binding energy that grows exponentially with \( U' \), something difficult to resolve even with a careful finite size analysis. Nevertheless, as \( U' \) is increased, we find an instability toward exciton formation such that they form a quasi-condensate with finite center of mass momentum, corresponding to an excitonic density wave (EDW). This can be understood through our analysis of the three-body problem of an electron-hole pair and a spinon: at quarter-filling, the system behaves basically
as a single doped \( t - J \) chain where the excitons act as holes hopping with both nearest, and next-nearest hoppings. These holes are heavier and can condensate, since they are electron-hole bound states in reality. In general, the period of this EDW will be determined by the excitonic fraction \( \frac{N_2}{L} \) (or \( \Delta \)). It is important to point out that this state corresponds to neither a CDW (or excitonic CDW), since there is no charge order, nor an FFLO-like phase, since the condensate wave function, or natural orbitals, alternates signs as \((++-\) like a square wave that has no poles, resulting in a density without nodes. However, this EDW can be directly related to pair density waves (PDW) \([170–172]\) in a very simple way: A particle-hole transformation in the high-energy orbital \( \lambda = 2 \) leads to a one-to-one correspondence between excitons (neutral particle hole pairs) and Cooper pairs (with charge \( 2e \)), with the excitonic condensate translating into a pair density wave. Accordingly, the parent Hamiltonian of this state would have negative \( U' \) and would pair electrons with momentum \( k_{F_1} \) and \(-k_{F_2}\), identical to what takes place in the FFLO phases of the negative \( U \) Hubbard chain \([196–199]\). Below quarter filling, EDW also presents except that its center-of-mass momentum is given by \( Q = k_{F_1} + k_{F_2} \) and can acquire a long wavelength when the difference is small.

As the interaction \( U' \) is increased further, the excitons become heavier and more localized enabling the exchange interaction to bind them into bound pairs. At the same time, we observe signatures of an instability towards a charge density wave of biexcitons, reminiscent of the idea of an excitonic crystal \([200, 201]\). However, biexcitons are not localized, and the period of the CDW is different from the period of the condensate. Since the charge gap vanishes, we conclude that this is not a CDW but a condensate of biexcitons. Just like above, the particle-hole transformation can map the biexcitonic condensate to a PDW of composite objects of charge \( 4e \) similar to predictions for stripe superconductors in Ref[202]. Note that this can also be understood in the hard-core bosons model if the singlet is mapped to hard-core boson: The biexciton condensate would correspond to a condensate of bosonic pairs with finite center-of-mass momentum in the dilute limit.
For large values of the parameters, the system phase separates in two different ways: (i). For large $U'$, the system splits into electron-rich and hole-rich domains; within each domain, each orbital forms a Mott-insulating Heisenberg chain. (ii). For small $U'$ and large $J$, we find the physics of two $t - J$ chains, that phase separates independently, as encountered in the phase diagram of the single-orbital problem [4]. Before this occurs, however, we find a regime around $J \sim 2t$ in which one orbital is metallic while the other one is a spin-gapped superconductor, an actual orbital selective paired state.

Below quater filling, the behavior of EDW with finite value of momentum $Q = k_{F_1} + k_{F_2}$ presents but no trace of biexcitonic physics can be identified in our exploration of parameter space. This requires more extensive study in the future.

Our model is much simpler than the full multi-orbital Hubbard model but displays rich physics with a number of phases that resemble the phenomenology of both cuprates and iron pnictide, encouraging us to expect that there is much to learn from multiorbital model that can guide our intuition toward a comprehensive picture of these complicated materials.
Chapter 6

Internal entanglement and correlation structure of the Kondo problem

The work presented in this chapter has been published in Phys. Rev. B 95, 95, 115106 (2017).

6.1 Background

The Kondo problem describes a magnetic impurity screened by the spin of conduction electrons around it, forming a collective singlet state [203, 204]. Its simplest formulation is through the so-called Kondo impurity model:

\[
H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J_K \vec{S}_{\text{imp}} \cdot \vec{S}_{r_0}
\]

where the \( \vec{S}_{\text{imp}} \) represents an \( S = \frac{1}{2} \) impurity embedded in a Fermi sea of noninteracting fermions. The Kondo interaction with a fermion at position \( r_0 \) is parameterized
by the coupling $J_K$. This problem is intrinsically one-dimensional, and several approaches, such as the numerical renormalization group (NRG) [205, 206], the Bethe ansatz [207, 208], take advantage of this low dimensionality.

Most of our understanding of the Kondo problem stems from renormalization group (RG) formalisms that yield a physical picture: As zooming out from the impurity and looking at it from afar [209], the physics is independent of the distance. This corresponds to an infrared (IR) fixed point, characterized by a single energy scale—the Kondo temperature $T_K$—and is described by a bound state formed by the impurity and the conduction electrons, the “Kondo singlet”. The associated wave function is typically characterized as a screening cloud (called “Kondo cloud”) centered at the impurity and decaying in distance with a characteristic range $\xi_K$ [210–215] that depends on $J_K$ (or $T_K$). Especially, if $J_K$ is much larger than the bandwidth $W$, corresponding to the strong coupling limit, the singlet is a tightly bound state formed by the impurity and a localized electron at $r_0$. Nozieres [216, 217] elegantly demonstrated that this fixed point can be described within Fermi liquid theory: The bound state becomes just a scattering center and the remaining conduction electrons that are decoupled from the impurity will simply behave as free fermions with their wave function modified by a phase shift $\delta = \frac{\pi}{2}$. Since breaking the singlet will raise the energy by $\frac{3}{2}J_K$, it has the effect of excluding electron/or holes from the $r_0$ and the fixed-point Hamiltonian must take the form

$$H' = -t \sum_{j=1}^{L} [c_{j+1,\sigma}^\dagger c_{j,\sigma} + H.c.] + \text{weak interaction}$$

As we reduce $J_K$, the impurity will become correlated with electrons farther and farther from it, meaning that the Kondo cloud becomes larger and larger. In a small system, at some point the Kondo cloud will not fit into the “box” and it cannot form: The singlet will extend to the entire volume, meaning that the impurity will couple mostly to one electron at the Fermi level. The coexistence of these two deeply conflicting pictures of the internal structure of the ground state requires us
to provide a coherent one to unveil the puzzle.

6.2 Model and Methods

To model the conduction electrons, we adopt a one-dimensional tight-binding chain with open boundary conditions of size $2L + 1$ ($L$ even) and the impurity connected to the site in the middle [210]. By a simple folding transformation [218, 219], it can be mapped onto an equivalent chain of length $L + 1$ and an impurity coupled to the first site ($r_0 = 0$):

$$H_{el} = -\sqrt{2}t \sum_{\sigma} (c_0^\dagger c_1 + H.c.) - t \sum_{i=1,\sigma} (c_i^\dagger c_{i+1,\sigma} + H.c.)$$

where $t$ is the hopping matrix element and is taken to be our unit of energy. This process can be illustrated in Fig.(6.1) and it effectively projects out an inactive orbital and reduced the effective degrees of freedom, since the antisymmetric (anti-bonding) electrons of the original problem decouple from the impurity and only the symmetric components need to be taken into account.

![Figure 6.1](image)

**Figure 6.1**: After the folding mapping, the system of size $2L + 1$ reduces to an equivalent semi-chain of length $L + 1$. In the strong coupling limit $J_K \to \infty$, it reduces to a product state of a spin singlet and a free tight-binding chain with one less site.
This problem can readily be solved with the density matrix renormalization group (DMRG) [69, 70, 173] and indeed, it has been studied in the literature, particularly focusing on the spatial correlations [212, 220], and the bipartite entanglement entropy [221]. In the following, we conducted DMRG simulation in systems of up to \( N = L + 1 = 63 \) orbitals at half filling, keeping the truncation error below \( 10^{-8} \), meaning that we need to keep up to 3000 DMRG basis states for real space simulations. When the impurity is absent, the eigenstates of the problem are \( |k\rangle = c_k^\dagger |\text{vac}\rangle \), with energies \( \epsilon_k = -2t \cos k \) and “momenta” \( k = \frac{\pi}{2L+2} j \) (\( j=1,3,5,\ldots,2L+1 \)).

### 6.3 Correlations in a Mixed state

Here we turn our attention to the entanglement between the impurity spin and the individual electronic wave functions, i.e. electronic wavefunction in real space or momentum space. This is a problem of two spins embedded in a bath formed by the rest of the conduction electrons, effectively in a mixed state obtained after tracing out all rest conduction electrons. This problem has attracted a great deal of interest in the quantum information community and is very seldom looked at in the condensed matter context [222–224]. In the following, we will adopt the measure concurrence to characterize the pairwise entanglement in the ground state of Kondo problem. In addition, we will also measure the quantumness of the correlation between impurity and specific electron by quantum discord.

### 6.4 Concurrence in the Kondo problem

A good point to start is by rewriting the ground state wave function in a form that takes into account the symmetries of the problem, isolating the contributions of the impurity spin and the orbital of interest. In the absence of magnetic field, the problem has time-reversal symmetry, so the ground state wave function acquires the
form:

\[ |g.s.\rangle = a_\ell (|\uparrow\rangle |2\rangle_\ell |\alpha_\ell,\uparrow\rangle + |\downarrow\rangle |2\rangle_\ell |\alpha_\ell,\downarrow\rangle) + b_\ell (|\uparrow\rangle |\downarrow\rangle_\ell |\beta_\ell,\uparrow\rangle + |\downarrow\rangle |\uparrow\rangle_\ell |\beta_\ell,\downarrow\rangle) + c_\ell (|\uparrow\rangle |\uparrow\rangle_\ell |\delta_\ell,\uparrow\rangle + |\downarrow\rangle |\downarrow\rangle_\ell |\delta_\ell,\downarrow\rangle) + d_\ell (|\uparrow\rangle |0\rangle_\ell |\gamma_\ell,\uparrow\rangle + |\downarrow\rangle |0\rangle_\ell |\gamma_\ell,\downarrow\rangle) \]

where the states \(|\alpha_\ell,\sigma\rangle, |\beta_\ell,\sigma,-\sigma\rangle, |\delta_\ell,\sigma\rangle\) and \(|\gamma_\ell,\sigma\rangle\) don’t include the single particle orbital \(c_{\ell\sigma}^\dagger\) and contain phases (signs) that are unimportant in the following discussion. The states \(|\sigma\rangle_\ell, |2\rangle_\ell\) and \(|0\rangle_\ell\) indicate the occupation of the single orbital, which could be in momentum space, real space, or some other representation. The coefficients \(a_\ell, b_\ell, c_\ell\) and \(d_\ell\) depend on the orbital \(\ell\) and the single particle basis.

To determine the entanglement between the impurity and orbital \(\ell\), we consider that it primarily originates from the spin degree of freedom and we can take trace over configurations that are empty or double occupied, yielding a projected wave function \(|\phi\rangle\) not containing the terms proportional to \(a_\ell\) and \(d_\ell\). This is a legitimate assumption, since the impurity only contains spin and no charge. In the basis \(|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\) and \(|\downarrow\downarrow\rangle\), both the reduced density matrix and the two-particle density matrix are identical

\[
\rho_{\alpha\beta,\alpha'\beta'} = \frac{1}{2} \langle \phi | c_{\ell\beta}^\dagger c_{\ell\alpha} c_{\ell'\alpha'} c_{\ell'\beta'} | \phi \rangle
\]

Furthermore, we can rewrite it explicitly using some correlation functions of density and spins

\[
\rho = \frac{1}{2} \begin{pmatrix}
\langle n_{imp} n_{\uparrow} \rangle & 0 & 0 & 0 \\
0 & \langle n_{imp} n_{\downarrow} \rangle & \langle S_{imp}^+ S_{\ell}^- \rangle & 0 \\
0 & \langle S_{\ell}^+ S_{imp}^- \rangle & \langle n_{imp} n_{\uparrow} \rangle & 0 \\
0 & 0 & 0 & \langle n_{imp} n_{\downarrow} \rangle
\end{pmatrix}
\]

where \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\) is the density operator \(S_i^+\) (or \(S_i^-\)) represents spin-raising (or spin-lowering) operator. Here the diagonal terms represent the density-density correlations and non-vanishing off-diagonal terms denote the spin-flipped terms between
the impurity and the electron of $\ell$ orbital. For the Kondo problem, we can introduce some identities:

\[
\langle N_{\text{imp}} n_{\ell \sigma} \rangle = \langle n_{\text{imp}} \uparrow n_{\ell \sigma} \rangle + \langle n_{\text{imp}} \downarrow n_{\ell \sigma} \rangle = \langle n_{\ell \sigma} \rangle
\]

\[
\langle S_{\text{imp}}^z n_{\ell \sigma} \rangle = \frac{1}{2}[\langle n_{\text{imp}} \uparrow n_{\ell \sigma} \rangle - \langle n_{\text{imp}} \downarrow n_{\ell \sigma} \rangle]
\]

which yield:

\[
\langle n_{\text{imp}} \uparrow n_{\ell \sigma} \rangle = \frac{1}{2} \langle n_{\ell \sigma} \rangle + \langle S_{\text{imp}}^z n_{\ell \sigma} \rangle
\]

\[
\langle n_{\text{imp}} \downarrow n_{\ell \sigma} \rangle = \frac{1}{2} \langle n_{\ell \sigma} \rangle - \langle S_{\text{imp}}^z n_{\ell \sigma} \rangle
\]

(6.2)

Since $\langle n_{\text{imp}} \uparrow n_{\ell \uparrow} \rangle = \langle n_{\text{imp}} \downarrow n_{\ell \downarrow} \rangle$ and $\langle n_{\text{imp}} \downarrow n_{\ell \uparrow} \rangle = \langle n_{\text{imp}} \uparrow n_{\ell \downarrow} \rangle$, we obtain that

\[
\langle S_{\text{imp}}^z n_{\ell \uparrow} \rangle = -\langle S_{\text{imp}}^z n_{\ell \downarrow} \rangle
\]

and

\[
\langle n_{\text{imp}} \uparrow n_{\ell \sigma} \rangle = \frac{1}{2} \langle n_{\ell \sigma} \rangle + \sigma \langle S_{\text{imp}}^z n_{\ell \sigma} \rangle
\]

\[
\langle n_{\text{imp}} \downarrow n_{\ell \sigma} \rangle = \frac{1}{2} \langle n_{\ell \sigma} \rangle - \sigma \langle S_{\text{imp}}^z n_{\ell \sigma} \rangle
\]

where $\sigma$ denote $\pm$ for up and down spins. If the SU(2) symmetry of the problem is assumed, the reduced density matrix can be further simplified

\[
\rho = \frac{1}{2}
\begin{pmatrix}
\frac{(n_{\ell \uparrow}) - \delta_{\ell}}{2} & 0 & 0 & 0 \\
0 & \frac{(n_{\ell \uparrow}) + \delta_{\ell}}{2} & -\delta_{\ell} & 0 \\
0 & -\delta_{\ell} & \frac{(n_{\ell \uparrow}) + \delta_{\ell}}{2} & 0 \\
0 & 0 & 0 & \frac{(n_{\ell \uparrow}) - \delta_{\ell}}{2}
\end{pmatrix}
\]
where $\delta_{\ell} = -2\langle S_{\text{imp}}^{z}n_{\ell\uparrow} \rangle = -2\langle S_{\text{imp}}^{z}S_{\ell}^{z} \rangle$ (for a singlet). To apply to the entanglement, we need to normalize it and obtain

$$\rho' = \frac{\rho}{\langle n_{\ell\uparrow} \rangle} = \frac{1}{4}(1 - \Delta)I + \Delta|s\rangle\langle s|$$

where $\Delta = \frac{\delta_{\ell}}{\langle n_{\ell\uparrow} \rangle}$ and $|s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ represents a spin singlet. Using the form of $|\phi\rangle$, these quantities can be expressed as

$$\langle n_{\ell\uparrow} \rangle = c_{\ell}^{2} + b_{\ell}^{2}, \quad \delta_{\ell} = b_{\ell}^{2} - c_{\ell}^{2}$$

The reduced density matrix $\rho'$ acquires the peculiar form of a so-called “Werner state” [224], whose concurrence and quantum discord are given by

$$C(\rho') = \max\{0, \frac{3\Delta - 1}{2}\}$$

and

$$Q(\rho') = \frac{1}{4}[(1 - \Delta)\log_{2}(1 - \Delta) + (1 + 3\Delta)\log_{2}(1 + 3\Delta) - 2(1 + \Delta)\log_{2}(1 + \Delta)]$$

, respectively. Since $\Delta$ depends on the spin-spin correlation between the impurity and orbital $\ell$, non-vanishing quantum correlation does not indicate the entanglement unless it is strong enough to overcome the PPT condition of separability. We want to evaluate the concurrence and quantum discord between the quantum impurity and conduction electrons $c_{\ell}$ in both real and momentum space. For this purpose, we use the noninteracting form of the wave functions (without the impurity) $c_{k} = \sum_{i}U_{ki}c_{i}$ and calculate the correlations between the localized spin and these orbitals that yield the coefficients of the wave function in momentum space:

$$a_{k} = \langle n_{\text{imp},\uparrow}n_{k\uparrow}n_{k\downarrow} \rangle, \quad b_{k} = \langle n_{\text{imp}}(1 - n_{k\uparrow})n_{k\downarrow} \rangle, \quad c_{k} = \langle n_{\text{imp}}n_{k\uparrow}(1 - n_{k\downarrow}) \rangle$$
6.4.1 Exact solution for $J_K \to \infty$

In the strong coupling limit $J_K \to \infty$, the electron at $r_0$ gets trapped to form a tightly bound state with the impurity and almost completely decoupled from the rest of the chain, i.e. the whole system becomes a product of spin singlet and a free tight-binding chain with one less site (as illustrated in Fig.(6.1)). In this case, we can determine the coefficients of the general ansatz of the ground state Eq.(6.1) (see plot in Fig.6.2) and calculate the concurrence and discord (see Fig.6.3 and Fig.6.5(a), respectively), using formulas provided by Luo. For $J_K \to \infty$, the entanglement between the impurity and the electron at $k_F$ vanishes. As for the associated discord, a finite-size scaling in Fig.6.5(c) shows that the discord remains finite in the thermodynamic limit.

![Figure 6.2: Coefficients of the wave function as a function of momentum $k$ in the strong coupling limit for finite $L$.](image)

6.4.2 Numerical results

For different values of $J_K$, we calculate the “concurrence distribution” which refers to the dispersion in momentum or energy of this quantity. Results for $C$ (for $N = L + 1 = 63$ electrons) are plotted in Fig.(6.3). It shows a clear and dramatic change of behavior for weak and strong coupling: For small $J_K$ the impurity is entangled
mostly to a single electron at the Fermi energy. As $J_K$ increases, it tends to get entangled to higher energy electrons and the entanglement with the electron at $\epsilon_F$ is continuously suppressed. Eventually, in the strong coupling regime, the impurity couples mostly to high energy electrons and decouples \textit{completely} from the electron at the Fermi level. There is a broad range of momenta around the Fermi level, where $C$ is identically zero and in the figure, it looks as though the impurity has carved a hole in the concurrence distribution. This is consistent with our previous exact solution.

\textbf{Figure 6.3:} Concurrence momentum distribution $C(k)$ between a Kondo impurity and the electrons in the Fermi sea for $N = L + 1 = 63$. The exact results corresponding to the limit $J_K \rightarrow \infty, L \rightarrow \infty$. $C(k)$ is symmetric about $k_F = \frac{\pi}{2}$.

The behavior of $C(k_F)$ and $C(r_0)$ are also shown in Fig.6.4(a) for two system sizes. Remarkably, the concurrence for the first site of the chain $r_0$ vanishes for small $J_K$. In other words, if the coupling is too weak, the first site is totally separable from the impurity; if the coupling is strong enough (larger than some critical value $J_K^c$), the PPT condition of separability can be overcome and electron at the first site gets entangled with the impurity. In addition, the results indicate that this critical $J_K^c$ increases with the system size. As for the concurrence for other site $r \neq r_0$ of the chain, they always remain zero, since these correlations are always weak and entanglement has monogamy (that is, a quantum system being entangled with another one limits its possible entanglement with a third system). Similarly,
we show the result of quantum discord distribution in momentum and real space for various $J_K$ in Fig.(6.5). The dependence of $Q(k_F)$ on $J_K$ indicates the quantum discord decreases as the coupling $J_K$ increases. If $J_K$ is strong enough, the quantum discord between the impurity and the conduction electrons at $\epsilon_k$ reduces drastically but remains nonvanishing for any finite value of $L$.

Figure 6.4: Concurrence between a Kondo impurity and the electron at momentum $k_F$ as a function of $J_K$ for system sizes $N = 23$ and $N = 63$. Results for the concurrence with the orbital at position $r_0$ are also shown. (b),(c) Excitation gaps above the ground state for $N = 23, 63$, respectively. The arrows indicate the points at which $C(k_F)$ vanishes.

6.5 Projected Natural Orbitals

In the following, we will try to disentangle the Kondo singlet from the rest of the Fermi sea. Generally, this should be described as a reduced density matrix, meaning it is a mixed state. But according to the above discussion, the impurity is presumably entangled to a *single* electron in some proper basis, all we need is to identify this electronic wave function. This can be done by considering a particular basis
Figure 6.5: Quantum discord $Q$ between a Kondo impurity and the electron in the Fermi sea. Panel (a) shows the momentum distribution, while panel (b) shows it in real space. Panel (c) shows the finite-size scaling of $Q$ in a logarithmic scale.

of “projected” natural orbitals. We define the “projected” single particle Green’s function as

$$\tilde{G}^\sigma_{ij} = -\langle S^z_{imp}\rho^\dagger_{\sigma i}c_{\sigma j}\rangle$$

whose eigenvectors give the natural orbitals (NOs)

$$|\alpha_n\rangle = \alpha_n^\dagger|vac\rangle$$

where, for simplicity, we have omitted the spin index. Unlike the single particle Green’s function, this projection will unambiguously yield a dominant single particle eigenstate: In terms of the natural orbitals, the ground state can assume the form
as

\[ |g.s.\rangle = \frac{1}{\sqrt{2}} [ |\uparrow\rangle \alpha_{0\downarrow}^\dagger - |\downarrow\rangle \alpha_{0\uparrow}^\dagger ] \prod_{n=1}^{N-1} \alpha_{n\uparrow}^\dagger \alpha_{n\downarrow}^\dagger |\text{vac}\rangle \]

\[ = \frac{1}{\sqrt{2}} [ |\uparrow\rangle \alpha_{0\downarrow}^\dagger - |\downarrow\rangle \alpha_{0\uparrow}^\dagger ] |FS'\rangle \]  \hspace{1cm} (6.3)

where the single particle states \( |\alpha_i\rangle \) are the natural orbitals. In this basis, the impurity spin forms a spin singlet with the natural orbital \( |\alpha_0\rangle \) but completely disentangles from a Fermi sea formed by the remaining orthogonal natural orbitals. This wave function is very similar to the one proposed by Yosida in the 60s [225, 226] and also to the one proposed by Bergmann in his artificial resonant state approach [213]. Without loss of generality, we can calculate the single particle Green’s function in this basis

\[ G_{ij}^\uparrow = \langle \alpha_{i\uparrow}^\dagger \alpha_{j\uparrow} \rangle = \begin{cases} 
\frac{1}{2} & i = j = 0 \\
1 & i = j = 1, 2, \cdots \\
0 & i \neq j
\end{cases} \]

Validity of this ansatz : If the NO-version Yosida wave function was rigorously correct, the bipartite von Neumann entanglement entropy between the singlet (impurity and the dominant natural orbital) and the rest of the conduction electrons, \( S = -Tr(\rho \log_2 \rho) \), where \( \rho \) is the two-particle reduced matrix of the singlet should be zero. However, our results in Fig.(6.6) show that \( S \) is small, particularly in the weak and strong coupling regimes. As expected, there is a residual entanglement with the rest of the electrons for intermediate values of \( J_K \sim 4t \) which are relevant to “Kondo box” physics [227–231]. In the thermodynamic limit, the RG flows toward the strong coupling regime where \( S \to 0 \) is expected. In general, this wave function can be treated as a very good approximation to the actual ground state by calculating the ground state energy variationally. In fact, it can yield the correct ground state energy with three and even up to four digits.
Figure 6.6: Concurrence with the dominant natural orbital, and von Neuman bipartite entanglement entropy between the singlet and the rest of the system.

6.6 Kondo Screening Length

It has been proposed that the size of the electron wave function that screens the localized spin $\zeta_K$ could be measured in mesoscopic devices [211, 211, 229, 230, 232, 233]. Its determination is a nontrivial task, since the wave function typically decays algebraically. However, one could identify this length with the typical system size at which the renormalization flow enters the strong coupling universal regime. In our case, the concurrence at $k_F$ plays the role of determining precisely this cutoff.

To justify these arguments, we look at the evolution of the spectrum with $J_K$, shown in Figs.6.4(b) and 6.4(c). The behavior of the energies as a function of $J_K$ bears a resemblance to the NRG spectrum as a function of system size. One can see levels that run parallel to each other: the state labeled by $\Delta_2$ corresponds to a particle-hole excitation in the Fermi sea $|FS'\rangle$ in Eq.(6.3) and the level spacing is determined by the system size [234], and independent of $J_K$. At small $J_K$, one can see that the low energy excitations $\Delta_1$ are being pushed up in energy. These are genuine excitations of the Kondo singlet, and determine the characteristic energy scale $T_K$. The crossover between the two regimes happens as the first excited eigenvalue “merges” with the single particle excitation. Even though this is not a sharp transition, there is an energy cutoff that is determined by the critical value $J_{K}^{*}(L)$ at which the concurrence vanishes as seen in Figs.6.4(a)-6.4(c) for two system sizes.
We can calculate the critical value $J_K^*(L)$ for different sizes $L$, and invert this dependence to obtain $\xi_K(J_K)$ as shown in Fig.(6.7). The overall dependence can be summarized very accurately in an exponential fit $\xi_K = 6.55 \exp(\frac{7.6}{J_K})$. Physically, the screening length should scale to $\xi_K = 1$ in the limit $j_K \to \infty$, since in that case the impurity is tightly bound with the electron at $r_0$. This is inconsistent with the fit, implying the possibility of other correlations to the prefactor

![Figure 6.7: Kondo screening length extracted from a finite-size analysis by using the concurrence as an “order parameter”. The dashed line corresponds to an exponential fit $\xi_K = 6.55 \exp(\frac{7.6}{J_K})$.](image)

### 6.7 Conclusion

In this chapter, we studied the internal entanglement and correlation structure of the ground state of the Kondo problem using concurrence and quantum discord, some measures from quantum information theory. Our results for the concurrence show that for small $J_K \sim \frac{W}{L}$, the impurity tends to get entangled with all conducting electrons, but mainly those around the Fermi level. For mesoscopic systems, this means the Kondo cloud does not have space to form since the the Kondo length is larger than the geometric size of the system. As $J_K$ increases, the impurity starts creating particle-hole excitations in the Fermi sea and will entangle to the electrons above the Fermi level, and to the holes below it. Most interestingly, for large enough
For $J_K$, the electrons around the Fermi level tend to disentangle from the impurity spin, oblivious to its presence as though the impurity were transparent. It means that the transition (actually a crossover) from weak to strong coupling regimes can be suitably measured by the concurrence with the state at $k_F$, which therefore can be employed as a quasi-order parameter to determine the transition point at which it becomes identically zero. Equivalently, it offers the means to measure the Kondo screening length. Although the system undergoes such a “transition” between impurity and the electron at $k_F$, they always remain quantum as indicated by the quantum discord.

On top of that, we proposed an approximate function, essentially a product of an entangled singlet composed of the dominant “projected” natural orbital and the impurity, and the rest of the conduction electrons denoted by $|FS\rangle$. As the entanglement entropy and concurrence indicate, this trial wavefunction becomes exact in the $J_K \to 0$ and $J_K \to \infty$ limit, where the disentanglement between the singlet and the rest of the conduction electrons become exact, and can provide an interpolation between them. Using this natural orbital basis, the DMRG simulation can be conducted with a dramatic high efficiency, even though the Hamiltonian will now involve long range terms [235]. This simplification rests on the fact that the ground state wave function is very close to a product state. It is important to notice that these natural orbitals are optimized only for the ground state, and not the excited states.

Using the concurrence, we have associated the Kondo screening length $\xi_K$ to a characteristic “size” of the natural orbital wave function. This quantity differs from the Kondo scaling length and corresponds to an intrinsic property of the wavefunction: Beyond this distance from the Kondo impurity, the physics is dominated by the boundary, with free fermions weakly correlated to the impurity that treat the Kondo cloud as a scattering center.

These results and the tools developed here provide new insight into the single impurity problem, and may guide future studies for a better understanding of heavy
fermion systems and the exhaustion problem, and efficient real-frequency impurity solvers for dynamical mean field theory calculations.
Bibliography


Appendix A

Local Rung Approximation (LRA) for polarons

In the Local Rung Approximation (LRA), the Mott insulating state $|\psi_0\rangle$ can be written as a product of localized singlet rung dimers $|S_i\rangle$, each being the ground state of the local rung Hamiltonian

$$H = -t_y \sum_{i,\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + h.c.) + U \sum_{\lambda} (n_{\lambda\uparrow} - \frac{1}{2})(n_{\lambda\downarrow} - \frac{1}{2})$$

This is a good approximation for $\frac{t_y}{t_x} = 2$, since the binding energy of a rung singlet is about 4 times lower than the energy of a leg singlet. In terms of the local basis $\{|2_1, 0_2, s\rangle = \frac{1}{\sqrt{2}}(|\uparrow_1, \downarrow_2\rangle - |\downarrow_1, \uparrow_2\rangle), |0_1, 2_2\rangle\}$, the local Hamiltonian can be represented as

$$\begin{pmatrix} U & -\sqrt{2}t_y & 0 \\ -\sqrt{2}t_y & 0 & -\sqrt{2}t_y \\ 0 & -\sqrt{2}t_y & U \end{pmatrix}$$
so the ground state energy and the associated state are
\[ E_0 = \frac{U - \sqrt{U^2 + 16t_y^2}}{2} \]
\[ |g_s\rangle = \frac{\sqrt{2} t_y}{\sqrt{4t_y^2 + E_2^2}} (|2_1, 0_2\rangle + |0_1, 2_2\rangle) + \frac{E_2}{\sqrt{4t_y^2 + E_2^2}} |s\rangle \equiv |S_i\rangle \]
with \( E_2 = \frac{U + \sqrt{U^2 + 16t_y^2}}{2} \). Following [] , we calculate the dispersions of the hole-doped polaron band

**Symmetric polaron–LRA1** : The symmetric polaron state at rung \( \ell \) is defined as
\[ |\ell\rangle = |S_1\rangle |S_2\rangle \cdots |b_{\ell\uparrow}\rangle \cdots |S_L\rangle \]
where \( |b_{\ell\uparrow}\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1, 0_2\rangle - |0_1, \uparrow_2\rangle) \). So the delocalized state for the polaron can be constructed as
\[ |\psi_1(k)\rangle = \frac{1}{\sqrt{L}} \sum_{\ell=1}^{L} e^{ik\ell} |\ell\rangle \]
From the Lehmann formula, we can obtain the dispersion \( \omega(k) \) for symmetric polaron
\[ \omega(k) = \langle \psi_0 | H | \psi_0 \rangle - \langle \psi_1(k) | H | \psi_1(k) \rangle - \mu \]
\[ = E_0 - \langle \ell | H_{\ell} | \ell \rangle - \langle \psi_1(k) | H(t_x) | \psi_1(k) \rangle - \frac{U}{2} \]
\[ = E_0 - t_y - t_x A(0) \cos k - \frac{U}{2} \]
where \( A(0) \) can be extracted from the matrix element \( \langle b_{\ell-1,\uparrow} | \langle S_\ell | H(t_x) | S_{\ell-1} \rangle | b_{\ell,\uparrow}\rangle \)
\[ A(0) = \frac{(1 + \frac{E_2}{2t_y})^2}{1 + (\frac{E_2}{2t_y})^2} \]
. This calculation uses the action of \( H(t_x) \) on the basis \( |S_{\ell-1}\rangle | b_{\ell,\uparrow}\rangle \)
The anti-symmetric polaron state at rung $ell$ is defined as

$$|\ell_t\rangle = |S_1\rangle|S_2\rangle \cdots |B_{\ell\uparrow}\rangle \cdots |S_L\rangle$$

where $|B_{\ell\uparrow}\rangle = \frac{1}{\sqrt{2}}(|\uparrow_1, 0_2\rangle + |0_1, \uparrow_2\rangle)$. The calculation is similar to the symmetric case and we can obtain the dispersion $\omega(k)$ for antisymmetric polaron

$$\omega(k) = \langle \psi_0 | H | \psi_0 \rangle - \langle \Psi_1(k) | H | \Psi_1(k) \rangle - \mu$$

$$= E_0 - \langle \ell_t | H | \ell_t \rangle - \langle \psi_1(k) | H(t_x) | \psi_1(k) \rangle - \frac{U}{2}$$

$$= E_0 - t_y - t_x A(\pi) \cos k + U$$